

# Optimal Transport for Non-Conservative Systems

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## Abstract

We study, in finite volume, a grand canonical version of the McKean–Vlasov equation where the total particle content is allowed to vary. The dynamics is anticipated to minimize an appropriate grand canonical free energy; we make this notion precise by introducing a metric on a set of positive Borel measures without pre-prescribed mass and demonstrating that the dynamics is a gradient flow with respect to this metric. Moreover, we develop a JKO–type scheme suitable for these problems. The latter ideas have general applicability to a class of second order non-conservative problems. For this particular system we prove, using the JKO–type scheme, that under certain conditions – not too far from optimal – convergence to the uniform stationary state is exponential with a rate which is independent of the volume. By contrast, in related conservative systems, decay rates scale (at best) with the square of the characteristic length of the system. This suggests that a grand canonical *approach* may be useful for both theoretical and computational study of large scale systems.

## 1 Introduction

This paper concerns the evolution and the convergence to equilibrium for a certain class of non-linear diffusion equations which may vaguely be described as of the McKean–Vlasov or Keller–Segel type. Such systems have been well studied in recent years; here the primary distinction will be that the total mass is not conserved locally in time but, rather, is globally determined by the analogue of a *Lagrange multiplier* which is known as the *chemical potential*. Secondly, we work in finite volume. This setting is arguably (see [3]) the physically sensible approach to the mathematical study of approximately homogeneous fluids described by these dynamics. Extensive behavior – static or dynamic – can only emerge as the infinite volume limit of finite systems where the total mass scales with the volume. In this context, the non-conservative setup (AKA grand canonical) has distinct advantages over its conservative (AKA canonical) counterpart. Indeed, as is quite well known (see, e.g., [3]) the latter generically has

relaxation times which scale with a power of the characteristic length of the system. Here, (under some lenient conditions on the initial data and parameter values) we demonstrate an exponential convergence to equilibrium with a rate that is uniform in the volume. Moreover, this will be proved under conditions where the driving functional relevant to the problem does not necessarily enjoy convexity properties.<sup>1</sup> Our proofs of this assertions – precise statements will be presented at the close of this section – requires the parallel development of a theory of *optimal transport* for non-conservative systems. In particular, as will be outlined in Section 2 below, this necessitates the construction of a distance between positive  $L^2$  functions (which, with additional labor, might be extended to general Borel measures). And, associated with this distance and dynamics – as presented in Section 2 – will be a JKO-type scheme [12], which constitutes the core of the proof.

Here it is remarked that, since the start of this research, there has been a parallel development of some of these ideas by e.g., Mielke and Liero (see [17] and references therein) in the context of reaction diffusion equations. However, for us, the construction of the abstract framework is only the preliminary step: our efforts culminate in tangible results for the system which will be described in Eq.(4). It is also worth noting that while the equation we will study is akin to a reaction diffusion system, the results we have obtained will not apply to these systems which, ultimately, *are* conservative. In particular, unless the overall density is already homogeneous, equilibrium times in reaction diffusion systems will be dominated by diffusive modes which necessitates that the relaxation times scale with the square of the characteristic length of the system. However, in the *grand canonical* (hence non-conservative) versions of these reaction diffusion systems it is anticipated that the convergence rates for uniform equilibria will be independent of the volume; similar considerations apply for the types of problems treated in, e.g., [2].

At this stage we must underscore some æsthetic limitations: While in conservative cases, the JKO *schemes* necessarily pertain to the dynamic, the distance involved is generally universal depending e.g., only on the ambient space. In the current cases, as will become clear, what emerges is that the distance itself apparently depends on

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<sup>1</sup>These results should be contrasted with several notable earlier works e.g., [2] which treat systems in *a priori* infinite volume and obtain exponential convergence to equilibrium with a rate which – necessarily – is uniform in volume. The aforementioned pertain to conservative systems with finite mass; in the absence of external constraints all mass would eventually drift away. So, in these works, mass is confined by an external potential which render the setting to an effectively finite-volume problem. Moreover, the curvature of the confining potential provides uniform convexity which drives the exponential convergence. Scaling (or linear response theory) immediately shows that the actual rate of convergence is the curvature itself which, in turn, is the square of the *effective* length-scale of the system. The curvature dependence of the rate is explicit in the statement of Theorem 2.1 in [2] (c.f. equation (2.8)).

the particulars of the dynamical equation. (A somewhat analogous situation – in mass conserved cases – was considered in [7].) Nevertheless we remark that even without the JKO scheme, the grand canonical approach to this general set of problems may have distinctive advantages over the canonical versions. In this regard, it should be noted that for the problems studied here, for a.e. value of the chemical potential, the steady state solutions of the two systems coincide. Thus, while exponential convergence uniform in volume is not to be expected in the high density phase, it is not too much to hope that in general the grand canonical systems equilibrate in a reasonable computational time frame. The corresponding conservative versions often appear to be computationally unviable.

The central focus of this paper concerns the analysis of an inhomogeneous version of the McKean–Vlasov equation in which matter can effuse into and out of the system. The usual conservative version can be derived in a variety of contexts; the original rendition presumably dates back to [18]. The non-conservative version also admits several derivations. For the purposes of this motivational section, we will provide, in Subsection 1.2, a common (sketch of a) derivation based on familiar interacting particle models. This has a distinctive advantage that it connects directly to the *thermodynamics* (free energetics) which underlie these evolutions. The latter, which can always be analyzed without recourse to dynamics, is the subject of Subsection 1.1 below. In the forthcoming subsections, there will be no pretense a complete mathematical analysis, however, a full derivation may emerge in some future work.

## 1.1 Motivation

Consider a function  $N(x, t)$  obeying the McKean–Vlasov dynamic

$$\frac{\partial N}{\partial t} = \triangle N + \nabla \cdot (N \nabla w_N) \quad (1)$$

where

$$w_N(x) := \int_{\mathbb{T}_L^d} W(x - y) N(y) dy.$$

It may be assumed without too much loss of generality that  $W(\cdot)$  depends only on the modulus of its argument. While a variety of ambient spaces are possible, for simplicity here and throughout this work, we will use  $\mathbb{T}_L^d$ , the  $d$ -dimensional torus of side length  $L$  as indicated above. The  $L^1$  norm of  $N$  is preserved in time and with  $\int_{\mathbb{T}_L^d} N dx =: \vartheta L^d$ , this is precisely the problem studied in [3]. As is well known (e.g., this is discussed in [21], especially Ch. 8) Eq.(1) is a gradient flow with respect to the Wasserstein distance for the (canonical) functional

$$\mathcal{F}_\vartheta(N) := \int_{\mathbb{T}_L^d} (N \log N - N) dx + \frac{1}{2} \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x - y) N(x) N(y) dx dy.$$

In the context of minima for  $\mathcal{F}_\vartheta$  and/or evolution according to Eq.(1) it is preferable that  $W$  satisfy a condition known as H–stability which, in the present setup, reads that for all  $m(x)$  with  $m(x) \geq 0$ ,

$$\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)m(x)m(y)dxdy \geq 0.$$

We take some time to recollect some results for the minimizers of  $\mathcal{F}_\vartheta(\cdot)$  all of which are proved in [3] but some of which date back to an earlier epoch: see [15], [13], [8], [9], [16], [11]. It is assumed throughout that  $W$  satisfies the H–stability condition. If  $\vartheta$  is sufficiently small,  $N \equiv \vartheta$  is the unique minimizer. When  $W$  is of positive type, implying convexity of  $\mathcal{F}_\vartheta(\cdot)$ , this actually holds for all  $\vartheta$ . Otherwise, the uniform state becomes (linearly) unstable at  $\vartheta = \vartheta^\sharp$  which is given by the maximum of the absolute value of the negative Fourier modes of  $W$ . However, under fairly general circumstances, the existence of non–uniform minimizers occurs at  $\vartheta = \vartheta_T < \vartheta^\sharp$ ; for  $\vartheta > \vartheta_T$ , the uniform state is no longer a global minimizer.

The grand canonical generalization of  $\mathcal{F}_\vartheta$  wherein the integral of  $N$  is not fixed is given by

$$\mathcal{G}_\mu(N) := \int_{\mathbb{T}_L^d} (N \log N - [N + \mu N])dx + \frac{1}{2} \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)N(x)N(y)dxdy \quad (2)$$

where  $\mu$  is called the *chemical potential*. Here it is seen that the H–stability condition is, for all intents and purposes, essential. (It is also worth noting that some of the older results alluded to above were actually established under the jurisdiction of this grand canonical functional.) Let us summarize without proof the essential results needed for the background of this work. For fixed  $\mu$ , the set of minimizers is non–empty. There are well defined upper and lower integrated densities associated with each  $\mu$  both of which are realized by elements in this set. These integrated densities are (both) strictly monotone and coincide for a.e.  $\mu$ . If  $\mu$  is sufficiently small then the uniform state is the unique minimizer. The density in the uniform state is given by  $M_0 = M_0(\mu)$  which satisfies the equation

$$M_0 = e^\mu e^{-wM_0} \quad (3)$$

where  $w = \int_{\mathbb{T}_L^d} W(x)dx$ . It is noted that  $N \equiv M_0$  is always a stationary state for  $\mathcal{G}_\mu(\cdot)$ , i.e., it satisfies the relevant Euler–Lagrange equation which is known in this context as the Kirkwood–Monroe equation [15].

In particular,  $N \equiv M_0$  remains the global minimizer till a point of discontinuity  $\mu_T$  is reached where the upper and lower densities do not coincide and, in fact, bracket  $\vartheta_T$ . For values of  $\mu$  greater than  $\mu_T$  the uniform density is no longer the minimizer and, at a strictly higher chemical potential,  $\mu_\sharp$  – the value of  $\mu$  such that  $M_0 = \vartheta_\sharp$  – the uniform state becomes linearly unstable.

The implication is that the non-uniform minimizer for  $\mathcal{F}_\vartheta(\cdot)$  at  $\vartheta = \vartheta_T$  is non-homogeneous e.g., a droplet and, probably, cannot be understood without first understanding the grand canonical version of the transition. Moreover, simulations of the canonical dynamics at  $\vartheta \sim \vartheta_T$  may require unmanageable computational time scales till a non-uniform minimizer is reached. See, e.g., [3] Theorem 2.11. But before such questions can be addressed for the grand canonical problem, a dynamic must be presented which corresponds to the functional  $\mathcal{G}_\mu(\cdot)$ . This is the topic of our next subsection.

## 1.2 Dynamics

While it is clear on general grounds that the “correct” equation for grand canonical dynamics involves the augmentation of Eq.(1) by inhomogeneous terms, the form of these terms is not particularly obvious. Moreover, the guiding principle is somewhat nebulous: The physics dictates an intrinsic uncertainty in  $\|N\|_{L_1}$ ; while this is well understood in equilibrium, it is not so clear how this uncertainty is supposed to propagate dynamically. The answer lies in the stipulation that the (nebulous) physics of this intrinsic uncertainty is equivalent, at the microscopic level, to the circumstances where individual particles can appear and disappear according to (a) the energetics of the complementary configuration and (b) a parameter, already mentioned, called the chemical potential.

Thus we turn to an interacting particle model which is discretized: On some  $A \subseteq \mathbb{R}^d$  (or the torus) we let  $\mathbb{A}_\varepsilon$  denote the intersection of  $A$  with the integer lattice  $\varepsilon\mathbb{Z}^d$  with spacing  $\varepsilon$ . To implement a continuum limit which is consistent with the limit in which the number of particles tends to infinity, the sites of  $\mathbb{A}_\varepsilon$  must have additional structure, e.g., represent cells which are copies of some  $C_\varepsilon$  which contain  $|C_\varepsilon|$  submicro-sites with  $|C_\varepsilon| \rightarrow \infty$  as  $\varepsilon \rightarrow 0$ . We may assume that the submicro-sites are at most singly occupied (usually vacant).

Consider first the conservative case. We consider  $n$  particles with  $n \propto |\mathbb{A}_\varepsilon| \approx \text{Vol.}(A)\varepsilon^{-d}$ . Consider a particle configuration on  $\mathbb{A}_\varepsilon$ . As far as the microscopic configurations – pertaining to dynamics and thermodynamics – are concerned, we may simply record the occupation numbers of each cell:

$$\mathbf{X} = (\eta_x \in \{0, 1, 2, \dots, |C_\varepsilon|\} \mid x \in \mathbb{A}_\varepsilon).$$

For the systems of interest, the *Hamilton function* is given by

$$H(\mathbf{X}) = \frac{1}{n} \sum_{(x,y)} W(x-y) \eta_x \eta_y.$$

Here, we are anticipating the mean-field limit which necessitates the  $n^{-1}$  scaling. The function  $W$  is regarded as a (continuous) function on  $\mathbb{R}^d$  – which is H-stable – and the sum takes place over distinctive pairs of cells in  $\mathbb{A}_\varepsilon$ .

Dynamics for the canonical ensemble are invented in order to leave invariant the canonical distribution

$$P(\mathbf{X}) \propto e^{-H(\mathbf{X})}.$$

Although there are many possibilities, the most obvious transition rates  $\mathbb{T}_{X:Y}$  which satisfy the conditions of *detailed balance* – namely  $P(\mathbf{X})\mathbb{T}_{X:Y} = P(\mathbf{Y})\mathbb{T}_{Y:X}$  – are given by

$$\mathbb{T}_{X:Y} = \Delta(\mathbf{X}, \mathbf{Y}) e^{\frac{1}{2}[H(\mathbf{X}) - H(\mathbf{Y})]}$$

where  $\Delta(\mathbf{X}, \mathbf{Y}) \in \{0, 1\}$  satisfies  $\Delta(\mathbf{X}, \mathbf{Y}) = \Delta(\mathbf{Y}, \mathbf{X})$  is some pertinent restriction on the allowed transitions. A convenient choice is to require  $\Delta$  to vanish unless  $\mathbf{X}$  and  $\mathbf{Y}$  agree at all cell-sites save a single neighboring pair where the relevant  $\eta$ 's differ only by unity. In other words, we only allow single particle hops.

We now envision the  $\varepsilon \rightarrow 0$ ,  $n \rightarrow \infty$  limit of these dynamics. Here, we make no claims to a rigorous derivation; we simply perform the analog of the calculations done in [20] for the Ising case wherein the Cahn–Hilliard and Cahn–Allen equations were acquired. I.e., we expand terms and, scaling time by  $\varepsilon^{-1}$  and neglecting correlations, we retain only the leading order in  $\varepsilon$ . As is not terribly difficult to show, the resultant equation for the particle density  $N$  at  $x \in A$  is given by  $\frac{\partial N}{\partial t} = \nabla^2 N + \nabla \cdot N \nabla w_N$ , i.e., exactly the McKean–Vlasov equation, Eq.(1).

Regarding this course of events as *satisfactory* as far as the canonical distribution is concerned, we may derive, in a similar fashion, a dynamic for the grand canonical ensemble. We thus consider the  $n$ -particle Hamiltonian to be augmented by a chemical potential term and cell-configurations  $\mathbf{X}$  with variable total particle content,  $n = n(\mathbf{X})$ . I.e.,

$$H(\mathbf{X}) = \frac{1}{n} \sum_{(x,y)} W(x-y) \eta_x \eta_y - n\mu.$$

We define transitions as previously but in addition we now allow for additional transitions:  $\Delta(\mathbf{X}, \mathbf{Y}) \neq 0$  for  $\eta_z(\mathbf{Y}) = \eta_z(\mathbf{X}) \pm 1$  so, explicitly, single particles can simply appear or disappear. The rate for the disappearance of a particle proceeds exactly as anticipated by the energetics while the rate for the spontaneous appearance of a particle is augmented by a factor of  $|\mathcal{C}_\varepsilon|^{-1}$ . This later condition, which is innate, tends to keep the *cell* occupation numbers of order unity. Now we may simply take the (informal)  $\varepsilon \rightarrow 0$  limit which automatically drives the average  $n$  to infinity proportional to  $\text{Vol.}(A)\varepsilon^{-d}$ . The result is a grand canonical dynamic:

$$\frac{\partial N}{\partial t} - \nabla^2 N - \nabla \cdot (N \nabla w_N) = -N e^{-\frac{1}{2}(\mu - w_N)} + e^{\frac{1}{2}(\mu - w_N)}. \quad (4)$$

The equation above is the subject of our analysis. It is here noted that  $N \equiv m_0$  is always a stationary solution. The purpose of this work is to show that under conditions

of sufficient thermodynamic stability for  $M_0$ , and suitable conditions on the initial density, the density converges to this uniform state exponentially with a rate that is *independent* of the volume.

### 1.3 Statements of Main Theorems

We conclude this section by stating our main result. Hereafter, we shall use the notation  $M_0$  to denote not only the numerical value but also the *stationary density* that is identically equal to this value; it is assumed that no confusion will arise.

We need a few preliminary definitions: For  $\kappa \in (0, \frac{1}{2})$  we define the set of functions

$$\mathcal{B}_\kappa = \{N : \mathbb{T}_L^d \rightarrow \mathbb{R} : \kappa M_0 < N < \frac{1}{\kappa} M_0\}.$$

Also, for  $\alpha > 0$  we define

$$v_\alpha = \sup_k |k|^\alpha |\hat{W}(k)|$$

and for a function  $Y$ ,

$$\|Y\|_{\mathcal{D}_2} = \sum_k k^2 |\hat{Y}(k)|.$$

The main theorem is as follows:

**Theorem 1.1** (Main Theorem) *Let  $W$  be an  $H$ -stable interaction kernel with finite range (i.e.,  $W$  vanishes outside a ball of finite radius around the origin which is assumed to be small relative to  $L$ ). Under the regularity assumptions that  $v_4 < \infty$  and  $\|W\|_{\mathcal{D}_2} < \infty$  let us suppose that  $M_0$  is sufficiently small so that the conclusion of Propositions 4.1 holds for some  $\kappa' < \frac{1}{2}$ . In addition, suppose the initial density  $N_0$  is in  $\mathcal{B}_{\kappa'}$  and  $\|\log N_0\|_{\mathcal{D}_2} < \infty$ .*

*Then we have that for all  $t$ ,*

$$\mathcal{G}_\mu(N_t) - \mathcal{G}_\mu(M_0) \leq [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)] e^{-\lambda^\dagger t}$$

*for some  $\lambda^\dagger > 0$ . Moreover, the same type of estimate holds for the  $L^2$ -squared difference with the stationary solution:*

$$\|N_t - M_0\|_{L^2}^2 \leq \frac{1}{\sigma} [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)] e^{-\lambda^\dagger t}$$

*for some  $\sigma > 0$ .*

Moreover we also have:

**Theorem 1.2** *The equation (Eq.(4)) induces a natural distance  $\mathbb{D}(\cdot, \cdot)$  defined, at least, on  $L^2$  Borel measures which are bounded below. Furthermore, there is a discretization scheme of the JKO-type associated with this distance which converges to*

the continuum evolution. In particular, we have exponential decay in  $\mathbb{D}(\cdot, \cdot)$ :

$$\mathbb{D}(N_t, M_0)^2 \leq \frac{1}{\sigma} [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)] e^{-\lambda^\dagger t},$$

where  $\lambda^\dagger$  and  $\sigma$  are the same as in the statement of the main theorem.

It is (re)emphasized that the convergence rate is uniform in volume; hence this result may be regarded as a requisite first step for the – as of yet unformulated – infinite volume study of these fluids.

## 2 Otto Distance & JKO

For many mass conserving parabolic PDE's – e.g., in particular Eq.(1) – the geometric picture uncovered in [19] (see also the book [1]) has provided indispensable theoretical insight as well as certain practical tools. However, for mass non-conserved cases, the generalization of these ideas and their corresponding connection to some version of optimal transportation has not been definitive. Here, with the tangibles provided by Eq.(4) along with the functional  $\mathcal{G}_\mu(\cdot)$  from Eq.(2) that this dynamic has a tendency to minimize, we may parallel and – to some extent – extend, the developments of [19]. (We refer also to [17].)

In this section we will lay out the Riemannian structure underlying our evolution equation by introducing an inner product on the space of measures and an associated distance. Indeed, it is this underlying structure which motivates and clarifies the eventual exponential convergence to equilibrium. Associated with a distance is a natural time discretization scheme, i.e., the JKO scheme, which we think of as an infinite dimensional analogue of an Euler scheme. In [12], minimizers of this scheme are used to yield an approximate (weak) discretization to the underlying evolution; there, the relation to the classical mass conserved transportation problem was used as a conduit between this scheme and the original evolution equation.

In our case, instead of recourse to an explicitly pre-formulated transportation problem, we shall content ourselves with a Benamou–Brenier description of the distance, i.e., it is realized as the infimum over a set of advective transportation possibilities. Further, we shall consider an *approximation* to the distance (over short times) wherein our analogue of the continuity equation shall be linearized at the initial density. It is with this approximate distance that we shall define our JKO-type scheme in the next section. Our ideology, at least in this work, is therefore that the underlying abstract Riemannian structure should be used as a guide to what is ultimately a very concrete approach. Thus we shall not provide too many rigorous foundations for our discussions in this section; the basic results establishing that we indeed have a reasonable distance can be found in Appendix B.



Our starting point is to consider a suitable collection  $\mathcal{B}$  of Borel measures on  $\mathbb{T}_L^d$ . For the purposes of the current work, the setting which leads to the most expedient developments is to consider measures given by a density which is uniformly bounded below and is also in  $L^2$ :

$$\mathcal{B} = \{\mu \text{ a Borel measure on } \mathbb{T}_L^d \mid \mu > 0, \mu \in L^2\}. \quad (5)$$

What is to follow is motivated by writing Eq.(4) in advective form. The transport velocity field, denoted by  $V$ , clearly takes the form <sup>1</sup>

$$V = -\nabla \Phi_N, \text{ with } \Phi_N := \frac{\delta \mathcal{G}_\mu}{\delta N} = \log N - \mu + w_N$$

The right hand side of Eq.(4) is obviously not identically zero. But, it is noted, it has the same sign as  $\Phi_N$ . Thus, we may rewrite Eq.(4) in the form:

$$\frac{\partial N}{\partial t} = \nabla \cdot (N \nabla \Phi_N) - \Omega_N \Phi_N. \quad (6)$$

Here

$$\Omega_N := \frac{N e^{-\frac{1}{2}(\mu - w_N)} - e^{\frac{1}{2}(\mu - w_N)}}{\log N - \mu + w_N} \quad (7)$$

is seen to be positive and tending to a definitive limit (which incorporates into the definition) if both numerator and denominator vanish. We regard Eq.(6) as the fundamental advective form for the inhomogeneous case. In particular, we will say that  $N$  is *advected* by  $Q$ , if it satisfies Eq.(6) with  $\Phi_N$  replaced by  $Q$  and with  $\Omega_N$  exactly as in Eq.(7).

For  $N \in \mathcal{B}$  let us consider the tangent space,  $\mathcal{T}_N$  at  $N$ . This is understood as the behavior at time  $t = 0$  of all trajectories in  $\mathcal{B}$  passing through  $N$  at  $t = 0$  i.e., possible values of  $\frac{\partial N}{\partial t}|_{t=0}$ . As in the mass conserved cases, these objects are in correspondence with potentials which advectively cause  $\frac{\partial N}{\partial t}$  to take on this value: Specifically, for  $M \in \mathcal{T}_N$  we may define  $Q = Q(M)$  to be the potential which satisfies the elliptic equation

$$M = \nabla \cdot (N \nabla Q) - \Omega_N Q. \quad (8)$$

For  $M_1, M_2 \in \mathcal{T}_N$  it is thus natural to define

$$g_N(M_1, M_2) = - \int_{\mathbb{T}_L^d} M_1 Q_2 dx = - \int_{\mathbb{T}_L^d} M_2 Q_1 dx := \langle \nabla Q_1, \nabla Q_2 \rangle_N. \quad (9)$$

And so, explicitly, we have

$$\langle \nabla Q_1, \nabla Q_2 \rangle_N = \int_{\mathbb{T}_L^d} N (\nabla Q_1 \cdot \nabla Q_2) + \Omega_N (Q_1 \cdot Q_2) dx \quad (10)$$

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<sup>1</sup>In traditional fluid mechanics, see, e.g., [22] it is the *positive* gradient of the velocity potential which produces the velocity field. We adhere to the convention used in [19] wherein it is the *negative* gradient.

which is akin to a Sobolev inner product (for potentials) on  $\mathbb{T}_L^d$ . It is manifest that  $g_N(\cdot, \cdot)$  is positive definite and therefore defines a requisite inner product for elements of  $\mathcal{T}_N$ .

Next, we will demonstrate that Eq.(4) can be envisioned as the gradient flow of  $\mathcal{G}_\mu(\cdot)$  with respect to this metric. First, let us use this metric  $g_N(\cdot, \cdot)$  to define a  $\mathcal{B}$ -gradient. Consider a simple functional on  $\mathcal{B}$  of the form

$$\mathcal{J}(B) = \int_{\mathbb{T}_L^d} J(B, x) dx$$

where, e.g.,  $\mathcal{J}$  is of class  $C^1$ . The directional (Gâteaux) derivative at  $N$  in the direction  $M$  is defined by

$$d\mathcal{J}(N; M) := \lim_{\varepsilon \rightarrow 0} \frac{\mathcal{J}(N + \varepsilon M) - \mathcal{J}(N)}{\varepsilon}$$

– when it exists – and is given explicitly by

$$d\mathcal{J}(N; M) = \int_{\mathbb{T}_L^d} \frac{\delta J}{\delta N}(N) \cdot M dx.$$

Therefore, by analogy with the finite dimensional cases, we use the metric to define the gradient via

$$d\mathcal{J}(N; M) := g_N(\nabla_{\mathcal{B}} \mathcal{J}, M).$$

In light of the explicit form of the directional derivative, we may identify  $\nabla_{\mathcal{B}} \mathcal{J}$  with the associated advective potential  $\frac{\delta J}{\delta N}$ .

This nearly completes the program. Consider a weakened version of Eq.(6) which in the current language reads

$$- \int_{\mathbb{T}_L^d} Q \frac{\partial N}{\partial t} dx = \langle \nabla Q, \nabla \Phi_N \rangle_N$$

for some test function  $Q$ . As above, we denote by  $M = M(Q)$  the solution of the advective equation Eq.(8). We remind the reader that in the above display,  $\Phi_N = \log N - \mu + w_N = \frac{\delta \mathcal{G}_\mu}{\delta N}$  and so this form of Eq.(6) can be written as

$$g_N(M, \frac{\partial N}{\partial t}) = -g_N(M, \nabla_{\mathcal{B}} \mathcal{G}_\mu) \quad ( = - \int_{\mathbb{T}_L^d} M \frac{\delta \mathcal{G}_\mu}{\delta N} ).$$

Or, informally, against the backdrop of the given  $g_N(\cdot, \cdot)$ ,

$$\frac{\partial N}{\partial t} = -\nabla_{\mathcal{B}} \mathcal{G}_\mu;$$

this then fully justifies the terminology “gradient flow”.

The above metric  $g(\cdot, \cdot)$  allows for a definition of distance between elements of  $\mathcal{B}$ . Foremost, for  $V_1, V_2 \in L^2$  which are *vector* valued, we may define the inner product akin to that for gradient fields

$$\langle V_1, V_2 \rangle_N := \int N(V_1 \cdot V_2) + \Omega_N(\mathbb{I}_\nabla(V_1)\mathbb{I}_\nabla(V_1)) dx \quad (11)$$

where

$$\mathbb{I}_\nabla(V) := (\Delta)^{-1}(\nabla \cdot V) + \kappa(V)$$

the first term of which, on  $\mathbb{T}_L^d$ , is certainly well defined and the second is an adjustable constant to provide some leeway in the forthcoming developments.

In what follows (and in general in these contexts) we will use a subscript of  $t$  to denote time dependence – not to be confused with a partial derivative. Then, for  $N_0, N_1$  in  $\mathcal{B}$  we may consider the set of vector fields which advectively drive  $N_t$  from  $N_0$  at  $t = 0$  to  $N_1$  at  $t = 1$  in such a way that  $\frac{\partial N_t}{\partial t}$  remains in  $L^2(\mathbb{T}_L^d \times (0, 1))$ :

$$\begin{aligned} \mathcal{V}(N_0, N_1) := \{V \in L^2(N_t) \mid \frac{\partial N_t}{\partial t} + \nabla \cdot (N_t V) = -\Omega_{N_t} \mathbb{I}_\nabla V \\ \text{with } N_{t=0} = N_0, N_{t=1} = N_1 \text{ and } \frac{\partial N_t}{\partial t} \in L^2\} \end{aligned} \quad (12)$$

where the above is actually under the proviso “for some choice of  $\kappa(V)$ ” and we underscore, explicitly, that  $V$  itself as well as  $\kappa(V)$  may depend on time.

We claim that the set  $\mathcal{V}(N_0, N_1)$  is non-empty since we may consider the straight line path  $N_t = (1-t)N_0 + tN_1$  and find a (time dependent) gradient field which drives  $N$  along this path. Indeed, here,  $\frac{\partial N_t}{\partial t}$  is given by  $N_1 - N_0$  which is in  $L^2$ . Now given a curve in  $\mathcal{B}$  indexed by  $N_t$ , we may consider the Hilbert space (for potentials) equipped with the inner product  $(\phi, \psi)_{N_t}$  given by  $\int_0^1 \langle \nabla \phi, \nabla \psi \rangle_{N_t} dt$ . Since  $N_t$  is bounded from below, it turns out that  $\Omega_{N_t}$  is also bounded below (c.f., Eq.(34)). Thus, the  $L^2$  norm of a potential  $\phi$  is bounded above by a constant times the norm induced by the Hilbert space. It then follows that (integration against)  $N_1 - N_0$  can be viewed as a bounded linear functional on the Hilbert space and so the required driving gradient field is existentiated by the Riesz Representation Theorem.

We now define the distance  $\mathbb{D}$  via

$$\mathbb{D}^2(N_0, N_1) = \inf_{V \in \mathcal{V}(N_0, N_1)} \int_0^1 \langle V, V \rangle_{N_t} dt, \quad (13)$$

or, equivalently, for  $V$ 's in  $\mathcal{V}_T(N_0, N_1)$  which drive  $N_0$  to  $N_1$  on  $[0, T]$ ,

$$\mathbb{D}^2(N_0, N_1) = \inf_{V \in \mathcal{V}_T(N_0, N_1)} T \int_0^T \langle V, V \rangle_{N_t} dt.$$

It can be demonstrated that  $\mathbb{D}^2(\cdot, \cdot)$  is indeed the square of a distance which separates points and that for all intents and purposes, any minimization program for  $\mathbb{D}^2(\cdot, \cdot)$  may be carried out by considering only those fields which are derived from a velocity potential. These results have been collected in Appendix B.

**Remark 2.1.** Here we emphasize that the existence of a distance between points in  $\mathcal{B}$  (and one may hope to presume all Borel measures on  $\mathbb{T}_L^d$ ) automatically defines an (abstract) optimal transport problem in this context: indeed, the explicit realization

of the distance as an infimum implies a transport problem wherein the “optimal path” minimizes the relevant functional. It is unfortunate that these problems have not been tied to an explicit Monge–Ampere or Kantorovich type formulation.

Having introduced the preceding metric structure on  $\mathcal{B}$  and demonstrated the gradient flow properties of Eq.(6) for the functional  $\mathcal{G}_\mu(\cdot)$  with respect to this metric, we may then consider the following JKO–type scheme:

$$N_{t+h} = \text{Argmin}\left\{\frac{1}{2}\mathbb{D}^2(N_t, N) + h\mathcal{G}_\mu(N)\right\} \quad (14)$$

which is a direct generalization of the scheme in [12] to these inhomogeneous cases.

### 3 The Approximate Functional

In this section we will proceed to construct an approximate functional whose minimizers will explicitly yield a discretization of our equation. It should be emphasized that JKO–type functionals, even when summed up over all iterations, do not admit a meaningful  $h$  tends to zero functional to be minimized – these are dissipative systems. In this sense, all such functionals are finite  $h$  “approximate”. Here for motivational purposes it is worthwhile to understand the difference between our situation and the mass conserved case as treated in [12]. In the latter, the *exact* approximate functional (e.g., as displayed in Eq.(14)) was employed. It was found that the minimizers were an approximate discretization converging to the relevant dynamics. To accomplish these ends, virtually all of the existing machinery of optimal transportation were deployed. This includes, but is not limited to: a well formulated and well studied underlying transportation problem, the coupled measure description for the Wasserstein distance, the pushforward formalism, a relation between the Wasserstein distance and variance, and, finally, the connection with the Brenier–Benamou description via transport fields.

The key difference here is that no such ancillary machinery has as of yet been developed for non–conservative problems. Indeed, *all* we have is the Brenier–Benamou formalism – which here defines the distance itself. Thus, instead of deploying the exact approximate functional, we shall use an *approximate* approximate functional whose *exact* minimizers provide a discretization. The principle difficulty in our approach is that the discretization arrived at is not as viable as the discretization acquired in [12] which (still only) approximated the minimizers. Hence, here, to obtain the  $h$  tends to zero limiting dynamics, an arduous, albeit elementary analysis is required. However, these technicalities can be neatly quarantined and is the subject of Appendix A.

### 3.1 Definition and Minimization

The starting point of our program entails a linearization of the distance itself (for small times). Let  $h > 0$  which we envision to be small and consider times  $0 \leq t \leq h$ . Let us replace the previously described distance functional by one where  $N_t$  is replaced in two crucial places by  $N_0$ . In particular, for all intents and purposes, under the auspices of  $h \ll 1$  we are replacing  $N_t$  with  $N_0$  in the inner product:  $\langle\langle \cdot, \cdot \rangle\rangle_{N_t} \rightarrow \langle\langle \cdot, \cdot \rangle\rangle_{N_0}$  and allowing this to inherit into the (approximate) dynamics. Starting with the latter, for fixed  $\phi$  we write

$$\frac{\partial N_t}{\partial t} = \nabla \cdot (N_0 \nabla \phi) - \Omega_{N_0} \phi. \quad (15)$$

Then the approximate distance is defined as

$$\mathbb{D}_A(N_0, N_h) := \inf_{\phi} \int_{\mathbb{T}_L^d} h \int_0^h [N_0 |\nabla \phi|^2 + \Omega_{N_0} \phi^2] dt dx$$

where under the above approximate dynamics,  $\phi$  gets us to  $N_h$  at time  $t = h$ . With  $\phi$  as argument (not necessarily minimizing anything) we will denote the right hand side by  $\mathbb{E}_A(\cdot)$ :

$$\mathbb{E}_A(\phi) := h \int_0^h \langle\langle \nabla \phi, \nabla \phi \rangle\rangle_{N_0} dt = \int_{\mathbb{T}_L^d} h \int_0^h [N_0 |\nabla \phi|^2 + \Omega_{N_0} \phi^2] dt dx.$$

Under reasonable conditions, we expect that for fixed  $N_0$  there is a unique *static* field which drives the system to  $N_h$  at time  $t = h$ . (See Eq.(16) in the statement of Proposition 3.2 below.) Since we will be utilizing Hilbert space structures, it is pertinent now to introduce notation for the relevant space of driving fields.

**Definition 3.1.** We let  $\mathcal{H}_{N_0}$  denote the Hilbert space (of driving fields) with the weighted inner product

$$\langle\langle \nabla \phi, \nabla \psi \rangle\rangle_{N_0} = \int_{\mathbb{T}_L^d} N_0 (\nabla \phi \cdot \nabla \psi) + \Omega_{N_0} \phi \psi dx.$$

The dual space will denoted by  $\mathcal{H}_{N_0}^{-1}$ .

Our first observation is that this static field actually minimizes the approximate distance functional:

**Proposition 3.2** *For fixed  $N_h - N_0 \in \mathcal{H}_{N_0}^{-1}$  and any driving field  $\phi$ , let  $\mathbb{D}_A(N_0, N_h)$  and  $\mathbb{E}_A(\phi)$  be as described. Then the minimum for  $\mathbb{D}_A(N_0, N_h)$  is achieved by the unique static  $\phi \in \mathcal{H}_{N_0}$  which satisfies*

$$\frac{N_h - N_0}{h} = \nabla \cdot (N_0 \nabla \phi) - \Omega_{N_0} \phi. \quad (16)$$

*Proof.* Since  $N_h - N_0$  is a bounded linear functional on  $\mathcal{H}_{N_0}$ , the existence (and uniqueness) of the required  $\phi$  again follows directly from the Riesz Representation Theorem.

Let us adapt the temporary notation  $N_t^{[\varphi]}$  for a density driven, according to the approximate dynamics, in the time interval  $0 \leq t \leq h$  by the field  $\varphi$ . A general driving field which achieves the desired  $N_h$  at  $t = h$  may be written in the form  $\phi + \alpha$  with  $\alpha$  (necessarily) depending on time. We have, weakly,

$$\begin{aligned} \frac{\partial}{\partial t} N_t^{[\alpha+\phi]} &= \nabla \cdot (N_0 \nabla (\phi + \alpha)) - (\phi + \alpha) \Omega_0 \\ &= \frac{\partial}{\partial t} N_t^{[\phi]} + \nabla \cdot (N_0 \nabla \alpha) - \alpha \Omega_0. \end{aligned} \quad (17)$$

It therefore follows that if  $\psi$  is a suitable time independent test function then

$$0 = \int_0^h \int_{\mathbb{T}_L^d} \psi [\nabla \cdot (N_0 \nabla \alpha) - \alpha \Omega_0] dx dt = - \int_0^h \int_{\mathbb{T}_L^d} [N_0 (\nabla \psi \cdot \nabla \alpha) + \psi \alpha \Omega_0] dx dt.$$

In particular, plugging in  $\phi$ , we have

$$\int_0^h \int_{\mathbb{T}_L^d} [N_0 (\nabla \phi \cdot \nabla \alpha) + \phi \alpha \Omega_0] dx dt = 0.$$

Now consider  $\mathbb{E}_A(\phi + \alpha)$ :

$$\mathbb{E}_A(\phi + \alpha) = h \int_0^h \int_{\mathbb{T}_L^d} N_0 [|\nabla \phi + \nabla \alpha|^2 + (\phi + \alpha)^2 \Omega_0] dx dt = \mathbb{E}_A(\phi) + \mathbb{E}_A(\alpha)$$

where, by the preceding display, the cross term has vanished. Since  $\mathbb{E}_A(\alpha)$  is positive, the desired result is established.  $\square$

**Definition 3.3.** Given a fixed  $N_0$ , let us now consider the JKO type functional associated with  $\mathbb{D}_A$ :

$$\mathbb{J}_A(N_0, N) := \frac{1}{2} \mathbb{D}_A^2(N_0, N) + h \mathcal{G}_\mu(N).$$

We make the observation that if  $N_0 \in \mathcal{B}$  then in fact  $N_0 \in \mathcal{H}_{N_0}^{-1}$ : Indeed, say  $N_0$  is bounded below by  $\kappa > 0$ , then by Eq.(34),  $\Omega_{N_0} \geq \sqrt{\kappa}$  and so if  $\phi \in \mathcal{H}_{N_0}$ , then  $|\int_{\mathbb{T}_L^d} N_0 \phi dx| \leq \|N_0\|_2 \|\phi\|_2 \leq \kappa^{-1/2} \|N_0\|_2 \|\phi\|_{\mathcal{H}_{N_0}}$ .

We first show that the functional  $\mathbb{J}_A(N_0, \cdot)$  can be minimized.

**Proposition 3.4** *Let  $N_0 \in \mathcal{B}$ . Then the functional  $\mathbb{J}_A(N_0, \cdot)$  has a minimizer in  $\mathcal{H}_{N_0}^{-1}$ . Furthermore, this minimizer is in  $L^1$ .*

*Proof.* For any  $N_0$ , we easily have that  $\mathbb{J}_A(N_0, \cdot)$  is bounded below. Explicitly, the function  $N \log N - (1 + \mu)N$  is minimized at  $N = e^\mu$  with value  $e^{-\mu}$  whereas the term involving  $W$  is positive by H-stability so (since we are in finite volume) the full free energy integral is bounded below. The distance term is of course positive.

Let us then take some minimizing sequence  $N^{(j)}$  in  $\mathcal{H}_{N_0}^{-1}$ . By the above observation, since  $N_0 \in \mathcal{B}$ , it is the case that  $N_0 \in \mathcal{H}_{N_0}^{-1}$  and so  $N^{(j)} - N_0 \in \mathcal{H}_{N_0}^{-1}$ . We now consider the driving fields  $\phi^{(j)}$  corresponding to  $N^{(j)}$  as given in Proposition 3.2 so that

$$N^{(j)} - N_0 = h(\nabla \cdot (N_0 \nabla \phi^{(j)}) - \Omega_{N_0} \phi^{(j)}). \quad (18)$$

Now

$$\mathbb{D}_A^2(N_0, N^{(j)}) = h \int_0^h \int_{\mathbb{T}_L^d} [N_0 |\nabla \phi^{(j)}|^2 + \Omega_{N_0} (\phi^{(j)})^2] dx dt$$

must be bounded since the free energy is bounded below and, further, the right hand side is just  $h^2$  times  $\langle \nabla \phi^{(j)}, \nabla \phi^{(j)} \rangle_{N_0}$ . We may therefore assert that along some further subsequence, if necessary,  $\phi^{(j)}$  converges weakly with respect to the inner product structure to some  $\phi^* \in \mathcal{H}_{N_0}$ . Let us next define  $N^*$  as the density corresponding to this  $\phi^*$ : we let  $N^* \in \mathcal{H}_{N_0}^{-1}$  be such that for all  $\psi \in \mathcal{H}_{N_0}$ ,

$$N^*[\psi] = \int_{\mathbb{T}_L^d} N_0 \psi dx - h \int_{\mathbb{T}_L^d} N_0 (\nabla \phi^* \cdot \nabla \psi) + \Omega_{N_0} \phi^* \psi dx.$$

On the basis of the weak convergence of the  $\phi^{(j)}$ 's we claim that the  $N^{(j)}$ 's have a weak limit (in  $\mathcal{H}_{N_0}^{-1}$ ) and that  $N^*$  is this limit. Indeed, letting  $\psi$  denote some suitable test function, we have

$$\begin{aligned} \lim_{j \rightarrow \infty} \int_{\mathbb{T}_L^d} N^{(j)} \psi dx &= \int_{\mathbb{T}_L^d} N_0 \psi dx - h \lim_{j \rightarrow \infty} \int_{\mathbb{T}_L^d} [N_0 (\nabla \psi \cdot \nabla \phi^{(j)}) + \Omega_{N_0} \psi \phi^{(j)}] dx \\ &= \int_{\mathbb{T}_L^d} N_0 \psi dx - h \int_{\mathbb{T}_L^d} N_0 (\nabla \phi^* \cdot \nabla \psi) + \Omega_{N_0} \phi^* \psi dx \end{aligned} \quad (19)$$

$$= N^*[\psi]. \quad (20)$$

(We remark that the above realization of  $N^*$  as a weak limit also implies that it is nonnegative.)

On the other hand, we claim that  $N^*$  is in fact (at least) an  $L^1$ -function: it was the case that  $\|N^{(j)}\|_{L^1}$  is uniformly bounded and in fact  $N^{(j)} \log N^{(j)}$  is integrable and its integral is uniformly bounded. Thus we assert that the associated measures converge vaguely and that the limit can be represented by an  $L^1$ -function which can then be identified with  $N^*$  (see for example the exposition in [4]).

We now claim that

$$\liminf_{j \rightarrow \infty} \mathbb{J}_A(N_0, N^{(j)}) \geq \mathbb{J}_A(N_0, N^*).$$

The lower semicontinuity of the terms involving  $N \log N - (1 + \mu)N + \mu$  and the  $\mathbb{D}_A^2(N_0, N)$  follow directly from convexity (indeed,  $\mathbb{D}_A^2(N_0, N^{(j)})$  is explicitly convex in the variables  $\phi^{(j)}$ ).

Now we address the interaction term. First note that for any function  $M$ , we have that

$$\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)M(x)M(y) \, dx dy = \frac{1}{L^d} \sum_k \hat{W}(k) |\hat{M}(k)|^2.$$

By the convergence of the  $N^{(j)}$ 's to  $N^*$ , it is clear that for any fixed  $k$ , we have that

$$\hat{N}^{(j)}(k) \rightarrow \hat{N}^*(k).$$

Let us obtain an *a priori* estimate for  $\hat{N}^{(j)}(k)$ : explicitly, we have that

$$(\hat{N}^* - \hat{N}^{(j)})(k) = -h \int_{\mathbb{T}_L^d} e^{ikx} \left[ ik \cdot N_0 ((\nabla \phi^* - \nabla \phi^{(j)}) + \Omega_{N_0}(\phi^* - \phi^{(j)})) \right] dx.$$

Taking absolute values and using Cauchy–Schwarz, we see that

$$|(\hat{N}^* - \hat{N}^{(j)})(k)| \leq G|k|$$

for some  $G < \infty$  (for  $k$  sufficiently large).

Now we apply the formula for the convolution displayed above to the quantity  $\int_{\mathbb{T}_L^d} (W * (N^* - N^{(j)}))(N^* - N^{(j)}) \, dx$  to show that it tends to zero: we obtain (dropping the factor of  $\frac{1}{L^d}$ )

$$\sum_k \hat{W}(k) |(\hat{N}^* - \hat{N}^{(j)})(k)|^2 = \sum_{|k| < k_0} \hat{W}(k) |(\hat{N}^* - \hat{N}^{(j)})(k)|^2 + \sum_{|k| \geq k_0} \hat{W}(k) |(\hat{N}^* - \hat{N}^{(j)})(k)|^2$$

for some fixed  $k_0 \gg 1$ . As  $j$  tends to infinity, the first term tends to zero. For the second term, using the estimate derived above, we are left with

$$\sum_{|k| \geq k_0} \hat{W}(k) |(\hat{N}^* - \hat{N}^{(j)})(k)|^2 \leq G^2 \sum_{k \geq k_0} k^2 |\hat{W}(k)|.$$

Since  $\|W\|_{\mathcal{D}_2} < \infty$ , the right hand side is the tail of a convergent sum and can be made arbitrarily small. We conclude that  $\lim_{j \rightarrow \infty} \int_{\mathbb{T}_L^d} (W * N^{(j)}) N^{(j)} \, dx = \int_{\mathbb{T}_L^d} (W * N^*) N^* \, dx$ .

It follows that

$$\inf\{\mathbb{J}_A(N_0, N), N \in \mathcal{H}_{N_0}^{-1}\} = \lim_{j \rightarrow \infty} \mathbb{J}_A(N_0, N^{(j)}) \geq \mathbb{J}_A(N_0, N^*)$$

and so indeed  $N^*$  is the minimizing element of  $\mathcal{H}_{N_0}^{-1}$ .  $\square$

While we cannot yet claim that  $N_h$  is uniformly bounded below, we do have:

**Proposition 3.5** *Let  $N_h \in \mathcal{H}_{N_0}^{-1} \cap L^1$  denote the minimizer of  $\mathbb{J}_A(N_0, \cdot)$  as given in Proposition 3.4. Then  $N_h$  is positive almost everywhere.*



*Proof.* Let  $N$  denote any nonnegative function for which  $\mathbb{J}_A(N_0, N)$  is finite and let

$$\mathcal{S}_0 = \{x : N(x) = 0\}.$$

If it were the case that  $\mathcal{S}_0$  has positive (Lebesgue) measure, then, we claim, it is possible to modify  $N$  so as to lower  $\mathbb{J}_A(N_0, \cdot)$ . Indeed, let  $n$  be a smooth positive function supported on  $\mathcal{S}_0$  with  $0 \leq n \leq 1$  and  $\int_{\mathcal{S}_0} n(x) dx = n_0 > 0$ . Now consider the modification  $N \mapsto N + \varepsilon n$  for some (small)  $\varepsilon > 0$ .

Now the key observation is that the effect of this modification on all terms contributing to  $\mathbb{J}_A(N_0, \cdot)$  *except* the entropy term (i.e., the  $N \log N$  term) is of order  $\varepsilon$ . For the distance squared term, note that e.g.,  $\mathbb{D}_A^2(N_0, N + \varepsilon n) \leq h^2(\|\phi\|_{\mathcal{H}_{N_0}} + \varepsilon\|\psi\|_{\mathcal{H}_{N_0}})^2$ ; here  $\phi$  is the driving field taking  $N_0$  to  $N$  and  $\phi + \varepsilon\psi$  is the driving field taking  $N_0$  to  $N + \varepsilon n$ ; c.f., proof of Proposition 3.6. The interaction term also has a linear (and quadratic)  $\varepsilon$  modification with bounded coefficients. Meanwhile,

$$\int_{\mathbb{T}_L^d} (N + \varepsilon n) \log(N + \varepsilon n) - N \log N dx = \int_{\mathcal{S}_0} n \varepsilon \log \varepsilon n dx \leq n_0 \varepsilon \log \varepsilon$$

which is negative and of considerably larger magnitude as  $\varepsilon$  tends to zero.

Thus, since  $N_h$  is a minimizer, the stated result follows.  $\square$

## 3.2 Discretization

We are now ready to show that successively running our JKO type scheme yields a discretization of our equation.

**Proposition 3.6** *Let  $N_h \in \mathcal{H}_{N_0}^{-1}$  denote the minimizer of  $\mathbb{J}_A(N_0, \cdot)$  as given in Proposition 3.4. Then  $N_0, N_h$  yield a weak discretization of the dynamics in Eq.(4). I.e., for all  $\psi \in \mathcal{H}_{N_0}$ ,*

$$\int_{\mathbb{T}_L^d} \frac{N_h - N_0}{h} \psi = - \int_{\mathbb{T}_L^d} N_0 (\nabla \Phi_{N_h} \cdot \nabla \psi) + \Omega_{N_0} \Phi_{N_h} \psi, \quad (21)$$

*i.e., weakly,*

$$N_h - N_0 = \nabla \cdot (N_0 \nabla \Phi_{N_h}) - \Omega_{N_0} \Phi_{N_h}. \quad (22)$$

*Further,  $\Phi_{N_h} \in \mathcal{H}_{N_0}$ .*

*Proof.* Let us denote by  $\phi \in \mathcal{H}_{N_0}$  the corresponding (static) field which drives the system from  $N_0$  to  $N_h$  in the time interval  $0 \leq t \leq h$  under the dynamics in Eq.(15), as given by Proposition 3.4 (the  $\phi$  here corresponds to the  $\phi^*$  in the proof of Proposition 3.4). Temporarily, letting  $\kappa > 0$ , we consider the variation  $N_h \mapsto N_h + \varepsilon h \eta$  with (bounded)  $\eta \in \mathcal{H}_{N_0}^{-1}$  that is supported on the set  $\{N_h(x) > \kappa\}$ .

Now there is a corresponding variation in the driving field which we denote by  $\varepsilon\psi$ , so that  $\phi \mapsto \phi + \varepsilon\psi$  “drives”  $N_0$  to  $N_h + \varepsilon\eta$ . Since the relevant equations are linear,  $\psi$  and  $\eta$  are simply related via

$$\eta = \nabla \cdot (N_0 \nabla \psi) - \Omega_{N_0} \psi \quad (23)$$

and so given  $\eta$ , the required  $\psi \in \mathcal{H}_{N_0}$  is given by Proposition 3.2.

Now to lowest order in  $\varepsilon$ ,

$$\mathcal{G}_\mu(N_h) \rightarrow \mathcal{G}_\mu(N_h) + \varepsilon \int_{\mathbb{T}_L^d} \eta \frac{\delta \mathcal{G}_\mu}{\delta N} dx = \mathcal{G}_\mu(N_h) + \varepsilon \int_{\mathbb{T}_L^d} \eta \Phi_{N_h} dx. \quad (24)$$

It is readily verified that all higher order terms divided by  $\varepsilon$  tend to zero as  $\varepsilon$  tends to zero (all coefficients are explicitly bounded since  $\eta$  is supported only where  $N_h > \kappa$ ).

Let us turn attention to the distance-type term. Here we have, exactly,

$$\begin{aligned} & \mathbb{D}_A^2(N_0, N_h + \varepsilon\eta) - \mathbb{D}_A^2(N_0, N_h) \\ &= - \int_{\mathbb{T}_L^d} (N_h + \varepsilon\eta - N_0)(\phi + \varepsilon\psi) dx - \int_{\mathbb{T}_L^d} (N_h - N_0)\phi dx \\ &= - \int_{\mathbb{T}_L^d} \varepsilon\eta\phi + \varepsilon(N_h - N_0)\psi dx - \varepsilon^2 \int_{\mathbb{T}_L^d} \eta\psi dx; \end{aligned}$$

it is clear that the  $\varepsilon^2$  term can be neglected. We now claim that the  $(N_h - N_0)\psi$ -term reproduces the  $\eta\phi$ -term: Indeed we have, from Eq.(16), that

$$\int_{\mathbb{T}_L^d} (N_h - N_0)\psi dx = h \int_{\mathbb{T}_L^d} [\nabla \cdot (N_0 \nabla \phi) - \Omega_{N_0} \phi] \psi dx = -h \langle \nabla \phi, \nabla \psi \rangle_{N_0}. \quad (25)$$

(The first equality in the above is understood weakly.) Since the inner product is symmetric, after a formal integration by parts, the role of  $\phi$  and  $\psi$  can be exchanged and we use the weak form of the elliptic equation defining  $\psi$  (as in Eq.(23)) to replace the expression involving  $\psi$  with  $\eta$ .

In combination with Eq.(24) we now see that the stationarity condition for the minimizer of  $\mathbb{J}_A(N_0, \cdot)$  yields

$$\int_{\mathbb{T}_L^d} \eta(\phi - \Phi_{N_h}) dx = 0.$$

This implies that  $\Phi_{N_h} = \phi$  on the set  $\{N_h > \kappa\}$ . By Proposition 3.5,  $\Phi_{N_h} = \phi$  a.e., since  $\kappa > 0$  can be made arbitrarily small. Since  $\phi \in \mathcal{H}_{N_0}$  we also conclude that  $\Phi_{N_h} \in \mathcal{H}_{N_0}$ .

Now to reproduce some discretization of the dynamics, we replace  $\phi$  by  $\Phi_{N_h}$  in Eq.(25) to obtain

$$0 = \int_{\mathbb{T}_L^d} \left( \frac{N_h - N_0}{h} \right) \psi + N_0(\nabla \Phi_{N_h} \cdot \nabla \psi) + \Omega_{N_0} \Phi_{N_h} \psi \, dx \quad (26)$$

for all  $\psi \in \mathcal{H}_{N_0}$ ; i.e., weakly, Eq.(22) is satisfied.  $\square$

For  $W$  of positive type, the overall  $\mathbb{J}_A(N_0, \cdot)$  is convex and uniqueness of  $N_h$  is guaranteed. In the more general circumstances of present interest, uniqueness will be established under the restrictive (presumably unnecessary) hypothesis that  $N_0$  is classical.

**Lemma 3.7** *If  $N_0 \in \mathcal{C}^1$  and bounded below, for  $h$  sufficiently small depending only on  $N_0$  and parameters of the theory (i.e.,  $W$ , assumed to be in  $\mathcal{C}_2$ ) there is a unique solution to Eq.(22) such that  $N \in L^1$  and  $\log N \in H^1$ .*

We note that the above implies in particular that the minimizer for  $\mathbb{J}_A(N_0, \cdot)$  from Proposition 3.6 is unique.

*Proof.* Let  $N_A, N_B$  denote two purportedly different solutions to Eq.(22). We define, using the notation of the Appendix,

$$\Psi_A = \log N_A = \log N_0 + h\psi_A$$

and similarly for  $B$ . In the  $\Psi$  variables, the (weak) equation takes on the form

$$\begin{aligned} N_A - N_B &= h[\nabla \cdot (N_0 \nabla (\Phi_{N_A} - \Phi_{N_B})) - \Omega_{N_0}(\Phi_{N_A} - \Phi_{N_B})] \\ &= h[\nabla N_0 \cdot (\nabla(\Psi_A - \Psi_B) + \nabla(W_{N_A} - W_{N_B})) + N_0(\nabla^2((\Psi_A - \Psi_B) + (W_{N_A} - W_{N_B}))) \\ &\quad - h\Omega_{N_0}((\Psi_A + W_{N_A}) - (\Psi_B + W_{N_B}))]. \end{aligned}$$

The cases where  $N_A - N_B \in L^\infty$  and  $N_A - N_B \notin L^\infty$  require slightly different treatments. First suppose  $N_A - N_B \in L^\infty$  and let  $m_{AB} = \|N_A - N_B\|_\infty$ . In the context of the  $L^\infty$  case we define

$$\mathcal{S} = \{N_A - N_B > \frac{m_{AB}}{2}\}, \quad (27)$$

where without loss of generality we may assume that this set is of positive measure.

For  $x \in \mathcal{S}$ , let us examine the difference of  $N_A$  and  $N_B$  subtracting a fraction  $hc_W$  from the left hand side where  $c_W$  is a constant to be determined shortly:

$$\begin{aligned} (1 - hc_W)(N_A - N_B) &= h\nabla \cdot (N_0 \nabla (\Psi_A - \Psi_B)) - h\Omega_{N_0}(\Psi_A - \Psi_B) \\ &\quad + h\nabla \cdot (N_0 \nabla (W_{N_A} - W_{N_B})) - h\Omega_{N_0}(W_{N_A} - W_{N_B}) - hc_W(N_A - N_B). \end{aligned} \quad (28)$$

(Here e.g.,  $W_{N_A} = W * N_A$ .) We claim that for properly chosen  $c_W$ , the terms on the second line of the above display total to a quantity which is pointwise negative, i.e.,

$$\begin{aligned} -h\mathbb{W}_{A,B} &:= -hc_W(N_A - N_B) + h\nabla \cdot (N_0 \nabla (W_{N_A} - W_{N_B})) - h\Omega_{N_0}(W_{N_A} - W_{N_B}) \\ &< 0. \end{aligned}$$

Indeed, for example, the term  $N_0 \nabla^2(W_{N_A} - W_{N_B})$  is easily bounded:

$$\begin{aligned} |N_0 \nabla^2(W_{N_A} - W_{N_B})| &= |N_0 \int_{\mathbb{T}_L^d} \nabla^2 W(x - y)(N_A(y) - N_B(y)) dy| \\ &\leq e^{||\Psi_0||_{\mathcal{C}_0}} m_{A,B} \|W\|_{\mathcal{C}_2}. \end{aligned}$$

The other terms are bounded proportional to  $m_{AB}$  as well. Now since  $x \in \mathcal{S}$ , we have  $N_A(x) - N_B(x) > \frac{1}{2}m_{A,B}$  and so by choosing  $c_W$  appropriately, the negative term  $-hc_W(N_A - N_B)$  can be made to compensate for any positive contributions from the other terms for  $c_W$  sufficiently large depending only on the particulars of  $W$  and  $N_0$ .

The fact that  $-\mathbb{W}_{A,B} < 0$  is pertinent to the remainder of the argument and establishing this negativity is the only essential reason for the distinction between the  $L^\infty$  versus not  $L^\infty$  cases. Let us now address the case where  $N_A - N_B \notin L^\infty$ : let  $H > 0$  be sufficiently large to be determined momentarily and here let us define

$$\mathcal{S} = \{N_A - N_B > H\}.$$

We claim that a modification of the preceding argument also shows  $-\mathbb{W}_{A,B} < 0$ : the terms involving  $W_{N_A}, \nabla W_{N_A}$  etc., will be estimated using the fact that  $W$  has only finite range  $-a$ . To this end let us define

$$M_a = \sup_{x \in \mathbb{T}_L^d} \int_{B_a(x)} |N_A(y) - N_B(y)| dy$$

where  $B_a(x)$  is the ball of radius  $a$  around  $x$ . ( $M_a$  is guaranteed to be finite since  $N_A - N_B \in L^1$ .) Since  $W(x - y)$  vanishes outside of  $B_a(x)$ , it follows that

$$|W_{N_A} - W_{N_B}| \leq \|W\|_\infty M_a.$$

Similarly estimates hold for the other terms and so for  $H$  sufficiently large depending on  $W$  and  $M_a$  the conclusion follows as before.

Next we transform Eq.(28) into  $\psi$  variables and we divide out  $(1 - hc_W)$  – assumed positive, which is certainly the case if  $h$  is sufficiently small:

$$\begin{aligned} e^{h\psi_A} - e^{h\psi_B} &= \frac{1}{1 - hc_W} \cdot [h^2[\nabla^2(\psi_A - \psi_B) + \nabla\Psi_0 \cdot \nabla(\psi_A - \psi_B)]] \\ &\quad - \frac{e^{-\Psi_0}}{1 - hc_W} [h\mathbb{W}_{A,B} + h^2\Omega_{N_0}(\psi_A - \psi_B)]. \end{aligned}$$

It is now noted that the last *two* terms on the right are pointwise negative and in fact in  $L^1$  if  $N_0$  is bounded below.

Next we consider the operator

$$\tilde{\mathbb{K}}_{N_0} = c_{N_0}\mathbb{I} - \Delta - \nabla\Psi_0 \cdot \nabla(\cdot)$$

It is claimed that for  $c_{N_0}$  sufficiently large depending only on  $N_0$ , the operator  $\tilde{\mathbb{K}}_{N_0}$  is positive in the sense that for any  $\varphi$  (e.g., in  $H^1$ ) we have  $\int_{\mathbb{T}_L^d} \varphi \tilde{\mathbb{K}}_{N_0} \varphi dx \geq 0$ . Indeed

$$\begin{aligned} \int_{\mathbb{T}_L^d} \varphi \tilde{\mathbb{K}}_{N_0} \varphi dx &= c_{N_0} \|\varphi\|_2^2 + \|\nabla\varphi\|_2^2 - \int_{\mathbb{T}_L^d} \varphi (\nabla\Psi_0 \cdot \nabla\varphi) dx \\ &\geq c_{N_0} \|\varphi\|_2^2 + \|\nabla\varphi\|_2^2 - \|\nabla\Psi_0\|_\infty \|\varphi\|_2 \|\nabla\varphi\|_2 \end{aligned}$$

and the claim is established for  $c_{N_0} > \frac{1}{4} \|\nabla \Psi_0\|_\infty^2$ . Now it will be required that  $h$  is sufficiently small depending on  $N_0$ , in particular  $hc_{N_0} < 1$ ,  $hc_W < 1$ .

We now write out the full difference equation for the  $\psi$ -variables:

$$(1 - hc_{N_0})(\psi_A - \psi_B) = \frac{-h}{1 - hc_W} \tilde{\mathbb{K}}_{N_0}(\psi_A - \psi_B) - \frac{1}{h} [\mathcal{E}_2(h\psi_A) - \mathcal{E}_2(h\psi_B)] - \frac{e^{-\Psi_0}}{1 - hc_W} [h\Omega_{N_0}(\psi_A - \psi_B) + \mathbb{W}_{A,B}],$$

where  $\mathcal{E}_2(x) := e^x - (1 + x)$ . It is noted, once again, that both terms on the bottom line of the above display are pointwise negative for  $x \in \mathcal{S}$ .

Redefining  $\mathbb{K}_{N_0} := [1 - hc_W]^{-1} [1 - hc_{N_0}]^{-1} \tilde{\mathbb{K}}_{N_0}$  the preceding equation now reads

$$(1 + h\mathbb{K}_{N_0})(\psi_A - \psi_B) = -\mathbb{P}_{A,B}$$

with  $\mathbb{P}_{A,B}(x) \geq 0$  for all  $x \in \mathcal{S}$ . Let us now write:

$$\psi_A - \psi_B = -[1 + h\mathbb{K}_{N_0}]^{-1} \mathbb{P}_{A,B}. \quad (29)$$

(Since  $\psi_A, \psi_B \in H^1$ , it is evident that  $\mathbb{P}_{A,B}$  is in the domain of the inverse operator.)

Let  $\varepsilon > 0$  which is envisioned to be small as will be specified later – but not vanishingly small. We claim that there is a subset of  $\mathcal{S}$  which is of nonzero measure such that  $|\psi_A - \psi_A^*| < \varepsilon$ ,  $|\psi_B - \psi_B^*| < \varepsilon$ ,  $|\mathbb{P}_{A,B} - \mathbb{P}_{A,B}^*| < \varepsilon$  for some values  $\psi_A^*, \psi_B^*, \mathbb{P}_{A,B}^*$ . Indeed, all that is required is the observation that e.g.,  $\mathcal{S} = \mathcal{S} \cap \cup_k \mathcal{S}_{A,k}$  where  $\mathcal{S}_{A,k} = \{x : \frac{2}{3}(k - \frac{1}{2})\varepsilon < |\psi_A| < \frac{2}{3}(k + 1)\varepsilon\}$ ; similar decomposition holds for the other quantities. So (up to a set of measure zero)  $\mathcal{S} = \mathcal{S} \cap (\cup_k \mathcal{S}_{A,k}) \cap (\cup_j \mathcal{S}_{B,j}) \cap (\cup_\ell \mathcal{S}_{\mathbb{P},\ell})$ . Since all unions are countable, there must exist  $k, j, \ell$  such that  $\mathcal{S}_{A,k} \cap \mathcal{S}_{B,j} \cap \mathcal{S}_{\mathbb{P},\ell}$  has nonzero measure. Let us denote this set by  $\mathcal{S}_\alpha$  and  $\chi_\alpha$  the indicator function of this set.

We will now integrate Eq.(29) on  $\mathcal{S}_\alpha$ :

$$\int_{\mathbb{T}_L^d} \chi_\alpha(\psi_A - \psi_B) dx = - \int_{\mathbb{T}_L^d} \chi_\alpha(1 + h\mathbb{K}_{N_0})^{-1} \mathbb{P}_{A,B} dx.$$

The left hand side is within  $\varepsilon$  of  $|\mathcal{S}_\alpha|(\psi_A^* - \psi_B^*)$ . The right hand side can be written as

$$- \int_{\mathbb{T}_L^d} \chi_\alpha \mathbb{P}_{A,B} dx + \int_{\mathbb{T}_L^d} \chi_\alpha \frac{h\mathbb{K}_{N_0}}{1 + h\mathbb{K}_{N_0}} \mathbb{P}_{A,B} dx.$$

The first term is within  $\varepsilon$  of  $-|\mathcal{S}_\alpha| \mathbb{P}_{A,B}^*$ ; as for the second term we note that the relevant operator is self adjoint and so

$$\begin{aligned} & \int_{\mathbb{T}_L^d} \chi_\alpha \frac{h\mathbb{K}_{N_0}}{1 + h\mathbb{K}_{N_0}} \mathbb{P}_{A,B} dx \\ & \leq \left[ \int_{\mathbb{T}_L^d} \left( \frac{h\mathbb{K}_{N_0}}{1 + h\mathbb{K}_{N_0}} \chi_\alpha \right)^2 dx \right]^{\frac{1}{2}} \left[ \int_{\mathcal{S}_\alpha} \mathbb{P}_{A,B}^2 dx \right]^{\frac{1}{2}} \leq |\mathcal{S}_\alpha|(\mathbb{P}_{A,B}^* + \varepsilon) \end{aligned}$$

where we have used that the operator norm of  $\frac{h\mathbb{K}_{N_0}}{1 + h\mathbb{K}_{N_0}}$  is less than 1. So the terms on the right hand side add up to no more than  $2\varepsilon|\mathcal{S}_\alpha|$ . The conclusion (by contradiction) is now clear since on the set  $\mathcal{S}$ , the quantity  $\psi_A - \psi_B$  is large e.g., compared to  $\varepsilon$ .  $\square$

### 3.3 Overview of the Iteration Scheme

We now provide the overview of how our JKO-type scheme is to be continued. Starting with some  $N_0$ , we define  $N_1 = \operatorname{argmin}\{\mathbb{J}_A(N_0, \cdot)\}$ ,  $N_2 = \operatorname{argmin}\{\mathbb{J}_A(N_1, \cdot)\}$ , etc. Of course in the present context, sufficient regularity of  $N_k$  (which hold by *fiat* for  $k = 0$ ) must be acquired in order to ensure that we can produce a unique  $N_{k+1}$ . More precisely, e.g., the abstract methods used so far only yield  $N_1 \in \mathcal{H}_{N_0}^{-1} \cap L^1$  and  $\log N_1 \in \mathcal{H}_{N_0}^1$  whereas in order to produce an  $N_2$  by these methods, we will actually need considerably more. The improved regularity will follow from suitably strong assumptions on  $N_0$  which will imply that  $N_1$  in fact coincides with a *classical* solution of Eq.(22), with well controlled norms. The detailed derivation of suitable estimates are the subject of Appendix A; let us summarize the setting of this appendix here:

- (a) The variables used in the appendix are logarithmic:

$$\Psi = \log N.$$

- (b) We employ “Fourier norms”:  $f \in \mathcal{D}_\ell$  means that the Fourier coefficients of the  $\ell^{\text{th}}$  derivatives of  $f$  are (absolutely) summable. These norms are discussed in a bit more detail in Section 5.2.

- (c) We assume that the initial  $\Psi_0$  is in  $\mathcal{D}_2$  and we also adopt an additional regularity assumption on the interaction potential, namely,

$$v_4 := \sup_k k^4 |\hat{W}(k)| < \infty.$$

(Typically, since  $W \in \mathcal{D}_2$ , one of these may be redundant, depending on dimension.)

We now summarize the logical steps entailed in the program:

**Step 1.** We assume  $\Psi_0 \in \mathcal{D}_2$  (and so  $N_0 \in \mathcal{B}$ ).

**Step 2.** We find  $N_1 = \inf \left\{ \mathbb{J}_A(N_0, N) : N \in \mathcal{H}_{N_0}^{-1} \right\}$  (see Proposition 3.4).

**Step 3.** By a variational argument, we conclude that  $N_0$  and  $N_1$  provides a one step time discretization of Eq.(4) and in fact  $\Phi_{N_1} \in \mathcal{H}_{N_0}$  (see Proposition 3.6).

**Step 4.** Since  $N_1$  satisfies the stationarity condition Eq.(22) and  $N_0, N_1$  satisfy the requisite conditions of Lemma 3.7,  $N_1$  is uniquely specified.

**Step 5.** Lemma 3.7 also implies that  $N_1$  coincides with the classical solution used in the Appendix and so particularly  $N_1 \in \mathcal{B}$  (see Corollary 5.4) and  $\Psi_1 \in \mathcal{D}_2$  and we may now repeat the previous steps to obtain  $N_2, N_3$ , etc. For any fixed  $k$ , this allows for the production of  $N_1, \dots, N_k$ , provided that  $h$  is sufficiently small.

**Step 6.** After  $k$  iterations, the macroscopic time achieved is only  $kh$  – thus vanishing with  $h$ . However, in Proposition 5.6 we achieve a guaranteed nonzero macroscopic time, i.e., for some fixed  $T > 0$  and all  $h$  sufficiently small, the process can be carried out for at least the order of  $h^{-1}T$  iterations.

**Step 7.** Via a comparison with the continuum solution, in Proposition 5.7 it is shown that the macroscopic time can be extended indefinitely; of course,  $h$  has to be suitably small depending on the prescribed time of simulation.

### 3.4 Convergence

Here we will show that the discretization scheme based on Eq.(22) indeed converges to a solution to Eq.(4). We reiterate: starting with some  $N_0$ , we define  $N_1, N_2, \dots$  as far as can be done. On occasion, we will denote  $N_k$ , the  $k^{\text{th}}$  iterate by  $N_t^{[h]}$  for time step  $h$  when  $k$  satisfies  $kh \leq t < (k+1)h$ ; it is in this context that we take the  $h \rightarrow 0$  limit.

Assuming that  $N_t^{[h]}$  exists for non zero  $t$  uniformly in  $h$ , the extraction of a weak limit is relatively easy; indeed, since each step of the iteration only lowers the free energy we have that  $N \log N$  is integrable and so a (subsequential) limit certainly exists. Further, limited results pertaining to continuity in time – Hölder-1/2 – can also be deduced from the structure implicit in the JKO type scheme, along the lines of what was done in [12]. However, these ideas do not suffice for a demonstration that the limiting object actually satisfies Eq.(4).

In order (to acquire enough control) to show that the limiting  $N_t$  satisfies the requisite equation, we have need for rather strong estimates, which we provide in the Appendix A using Fourier methods. The analysis in Appendix A is performed essentially in the context of classical solutions, but, by the uniqueness statement in Proposition 3.6, this solution will coincide with the minimizer of the iterative scheme. The setting for Appendix A was summarized in the previous subsection.

For the purposes of the next theorem, let us use the notation  $[\cdot]_t^{[h]}$  for the various quantities encountered.

**Theorem 3.8** *Let  $T > 0$  be arbitrary (so that the iterative process is suitably valid for all  $h < h_T$  with  $h_T$  as in Proposition 5.7). Letting  $\Psi_t^{[h]} = \log N_t^{[h]}$ , we have that  $\Psi_t^{[h]}$  converges to a weak solution,  $\Psi_t$ , of Eq.(4) (written in these logarithmic variables) as  $h$  tends to zero. Moreover,*

(A) *This convergence is, in fact, strong in the  $\mathcal{D}_1$ -norm and uniform in the  $\mathcal{D}_0$ -norm.*

(B)  *$N_t = e^{\Psi_t}$  is the unique solution to the continuous time equation as given by Eq.(4) which is  $\mathcal{C}^\infty$  for positive times and  $N_t \rightarrow N_0$  strongly in  $\mathcal{D}_0$  as  $t \rightarrow 0$ .*

*Proof.* Item (A) will be established in Appendix A after the proof of Proposition 5.7 and Item (B) will be addressed briefly at the end of the proof. Let us now establish the main convergence result.

We will first establish that if  $N_t$  is a weak limit of  $N_t^{[h]}$  as  $h$  tends to zero, then  $N_t$  is a weak solution to Eq.(4). (It is clear, e.g., from the discussion before the statement

of this theorem that one can always extract a weak limit.)

Now consider a sufficiently smooth test function  $b(x, t)$  supported on  $(0, T)$  (e.g.,  $b \in \mathcal{C}^1((0, T) \times \mathbb{T}_L^d) \cap L^\infty$ ) which is integrated against both sides of the iteration equation as in Eq.(21) then summed over the order of  $Th^{-1}$  iterations (recall that  $\Phi_t^{[h]} = \Psi_t^{[h]} - \mu + w_{N_t^{[h]}}$ ):

$$\begin{aligned} & \sum_k \int_{\mathbb{T}_L^d} \left( \frac{N_{k+1} - N_k}{h} \right) b dx = \\ & - \sum_k \int_{\mathbb{T}_L^d} N_k [\nabla(\Psi_{k+1} + w_{N_{k+1}}) \cdot \nabla b] + \Omega_{N_k} [\Psi_{k+1} - \mu + w_{N_{k+1}}] b dx. \end{aligned} \quad (30)$$

The left hand side, after summation by parts, weakly converges to the integral of  $-N_t^{[h]}(\partial b / \partial t)$ . As for the right hand side, first for notational convenience we will write e.g.,  $N_t^{[h]}$  instead of  $N_k$  and  $N_{t+h}^{[h]}$  instead of  $N_{k+1}$  and then the sum over  $k$  can be replaced by an integral over  $[0, T]$ . First we observe that if it were the case that all the indices were in agreement and equal to  $k+1$ , then the right hand side can be realized entirely as a weak equation for  $N_t^{[h]}$  (with most of the burden of differentiation passed on to  $b$ ) which would converge weakly to the relevant limit. What we must estimate then is the differences caused by the discrepancy in indices. For example, in the term containing  $\Psi$ , forcing the indices to match yields the residual term

$$- \int_0^T \int_{\mathbb{T}_L^d} (N_{t+h}^{[h]} - N_t^{[h]}) (\nabla \Psi_{t+h}^{[h]} \cdot \nabla b) dx dt.$$

By the results obtained in Appendix A (see Corollary 5.8) we have that  $|\nabla \Psi_t^{[h]}|$  is uniformly bounded – e.g., in  $L^\infty$  – in both  $h$  and  $t$  while  $N_{t+h}^{[h]} - N_t^{[h]} = e^{\Psi_{t+h}^{[h]}} - e^{\Psi_t^{[h]}}$  is bounded above by  $h$  times a function which, again, has a uniform  $L^\infty$  bound. Hence, this error term disappears from consideration in the  $h \rightarrow 0$  limit.

Identical considerations apply to the term  $N_t^{[h]}(\nabla w_{N_{t+h}} \cdot \nabla b)$ . However, here, the situation is even less demanding since  $\nabla w_N$  does not even involve gradients of  $\Psi$ . As for the inhomogeneous term, it is slightly easier to do the reindexing on the  $\Phi$ -terms. We write

$$\Phi_{t+h}^{[h]} \Omega_t^{[h]} = \Phi_t^{[h]} \Omega_t^{[h]} + (\Phi_{t+h}^{[h]} - \Phi_t^{[h]}) \Omega_t^{[h]}.$$

The leading term on the right of the above display is of the correct form. Examining the definition of  $\Omega_N$ , it is clear that if  $\Psi$  is bounded (e.g., in  $L^\infty$ ) then so is  $\Omega_N$ . Since  $\Phi_N = \Psi_N + w_N - \mu$ , we have that  $|\Phi_{t+h}^{[h]} - \Phi_t^{[h]}|$  is bounded by order  $h$  and this term also disappears in the  $h \rightarrow 0$  limit.

Finally, by standard regularity results about (uniformly) parabolic equations, we have that  $N_t$  is smooth ([5]) for positive times and the convergence to initial data can be easily gleaned from the results in Appendix A.  $\square$



## 4 Proof of the Main Theorem

In this section, we provide a proof of the principal *result* of this work. Namely: If the initial  $N_0$  is in the vicinity of the uniform state, and the latter is “sufficiently stable” then the subsequent dynamics is characterized by exponential convergence to this state.

### 4.1 Convexity Estimates

In this subsection, we aggregate all the results concerning *convexity* of the function  $\mathcal{G}_\mu(\cdot)$  which will be used in the proof of the main theorem. First, it is seen that if  $W$  is of positive type then  $\mathcal{G}_\mu(\cdot)$  is always convex for all values of  $\mu$ . But, it is also known that such circumstances also foreclose any possibility of a phase transition. However, even here, the rate of convergence to equilibrium is still of interest. More pertinently in the general cases, it is not unreasonable to assume that if  $e^\mu$  is sufficiently small *and* overall the fluid is reasonably homogeneous with a density not too far from the uniform state that some local convexity properties should ensue.

First, recall the definition of (the density of) the uniform state  $M_0$  which is the solution to  $M_0 = e^{\mu - M_0 w}$  with  $w$  being the integral of  $W$ , as described following Eq.(3). In what follows, instead of using  $\mu$  – which is ostensibly large and negative – as our parameter we will use the quantity  $M_0 = M_0(\mu)$  as our (small) parameter.

**Proposition 4.1** *Let  $\kappa$  be any number  $0 < \kappa < \frac{1}{2}$  and suppose that at time  $t_0 \geq 0$  the density  $N_{t_0}$  satisfies the pointwise bounds*

$$\kappa M_0 < N_{t_0}(x) < \frac{1}{\kappa} M_0.$$

*Then, if  $M_0$  is sufficiently small, this condition persists for all time  $t > t_0$ .*

*Proof.* Examining Eq.(4) and recalling we can reason classically, let us assume that  $x_\sharp$  is a point of maximum or minimum. Then at  $x = x_\sharp$ , we have

$$\frac{\partial N_t(x_\sharp)}{\partial t} \geq N \nabla^2 w_{N_t} - (N_t e^{-\frac{1}{2}(\mu - w_{N_t})} - e^{+\frac{1}{2}(\mu - w_{N_t})})$$

for a minimum and with the opposite inequality if  $x_\sharp$  is a maximum.

Now we claim that for  $M_0$  sufficiently small,

$$-\kappa M_0 e^{-\frac{1}{2}(\mu - w_{N_t})} + e^{+\frac{1}{2}(\mu - w_{N_t})} \geq \kappa M_0^{\frac{1}{2}}$$

and

$$-\frac{1}{\kappa} M_0 e^{-\frac{1}{2}(\mu - w_{N_t})} + e^{+\frac{1}{2}(\mu - w_{N_t})} \leq -M_0^{\frac{1}{2}}.$$

Indeed, the second display amounts to the inequality  $e^{\frac{1}{2}(w_{N_t} - w_{M_0})} - \kappa e^{-\frac{1}{2}(w_{N_t} - w_{M_0})} \geq \kappa$  and we can use  $w_{N_t} \geq -\frac{1}{\kappa} M_0 w_0$  while the first display reduces to  $e^{\frac{1}{2}(w_{M_0} - w_{N_t})} -$

$\kappa e^{-\frac{1}{2}(w_{M_0}-w_{N_t})} \geq \kappa$  and we can also use  $w_{N_t} \leq \frac{1}{\kappa}M_0w_0$ . The claimed result is now manifest for  $M_0$  sufficiently small.

Let us suppose then that at some time  $t_\sharp$ , for the first time, the density achieves the value  $\frac{1}{\kappa}M_0$  and this occurs at the point  $x = x_\sharp$  – which is its maximum. Then we would have

$$\frac{\partial N_{t_\sharp}(x_\sharp)}{\partial t} \leq -M_0^{\frac{1}{2}} + \frac{1}{\kappa}M_0w_2$$

which is strictly negative for  $M_0$  sufficiently small. While this immediately implies that at the point  $x_\sharp$ , the density can grow no bigger, it actually implies, by continuity, that such happenstance could never occur in the first place: At  $t = t_\sharp^-$  before the density at  $x = x_\sharp$  achieved  $\frac{1}{\kappa}M_0$ , the derivative was already negative.

Similar considerations apply – for  $M_0$  sufficiently small – if we investigate the first time that the density has fallen as low as  $\kappa M_0$   $\square$

Consider, then, the convex set  $\mathcal{B}_\kappa \subseteq \mathcal{B}$  consisting of those densities which satisfy the bounds featured in Proposition 4.1. (It is noted that the parameters of the upper and lower bounds need not be related. However, the condition is natural for the variable  $\Psi = \log N$ .) Our next claim is that if  $\kappa M_0$  is sufficiently small then the functional  $\mathcal{G}_\mu(\cdot)$  restricted to  $\mathcal{B}_\kappa$  is convex:

**Proposition 4.2** *For  $M_0/\kappa < \vartheta^\sharp$  where*

$$\frac{1}{\vartheta^\sharp} = \max_k \{|\hat{W}(k)| \mid \hat{W}(k) < 0\},$$

*the functional  $\mathcal{G}_\mu(\cdot)$  restricted to  $\mathcal{B}_\kappa$  is convex. And, therefore,  $N \equiv M_0$  is the unique minimizer in  $\mathcal{B}_\kappa$ . In the above we may take  $\vartheta^\sharp = \infty$  if the interaction is of positive type.*

*Proof.* Let  $N_A, N_B$  be temporary notation for densities in  $\mathcal{B}_\kappa$  and similarly, let us define  $N_s := (1-s)N_A + sN_B$  and  $R := N_B - N_A$ . A direct calculation shows

$$\frac{d^2 \mathcal{G}_\mu(N_s)}{ds^2} = \int_{\mathbb{T}_L^d} \frac{R^2}{N_s} dx + \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y) R(x) R(y) dx dy.$$

The first term on the right is larger than  $[\kappa/M_0] \|R\|_{L^2}^2$  and as for the second, we have

$$\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y) R(x) R(y) dx dy = \frac{1}{L^d} \sum_k \hat{W}(k) |\hat{R}(k)|^2 \geq -\frac{1}{\vartheta^\sharp} \|R\|_{L^2}^2$$

and the primary statement is proved. The secondary statement is immediately clear since  $N \equiv M_0$  is always a stationary point and the convexity that was just proved is actually strict.  $\square$

**Remark 4.3.** We remark that notwithstanding factors of order unity – e.g.,  $\kappa$  – the estimates here (and presumably those in Proposition 4.1) are reasonably sharp. Indeed,  $M_0 = \vartheta^\sharp$  is the point where the stationary solution  $N_t \equiv M_0$  is *linearly* unstable and, translating the results of [3] to the current context, when  $M_0 = \vartheta_T < \vartheta^\sharp$ , already there are non-trivial minimizers for  $\mathcal{G}_\mu(\cdot)$ .

## 4.2 Proof of Main Theorem

*Proof.* Let  $t > 0$  and  $T > t$ . Let  $\kappa > \kappa'$  and consider  $h$ 's sufficiently small so that throughout  $(0, T)$ , the actual  $N_t$  and  $N_t^{[h]}$  differ only slightly in e.g., the  $\mathcal{D}_1$ -norm. Thus, we may rest assured that for all  $t \in [0, T]$ , we have  $N_t^{[h]} \in \mathcal{B}_\kappa$  and that the conclusions of the above proposition hold with  $\kappa'$  replaced by  $\kappa$ .

In the following, we will examine one iteration of the process at fixed  $h$ . To avoid clutter, we will again employ the (inconsistent) notation that  $N_0$  is the initial density and  $N_1$  is the final density for this step. Let us define, for  $\lambda > 0$

$$M_\lambda^{(0)} := (1 - h\lambda)N_0 + h\lambda M_0$$

so that  $M_\lambda^{(0)} - N_0 = h\lambda(M_0 - N_0)$ . Let us also define  $Q$  to be the potential which pushes  $N_0$  all the way to  $M_0$  in unit time under the approximate dynamics:

$$M_0 - N_0 =: \nabla \cdot (N_0 \nabla Q) - \Omega_{N_0} Q.$$

Further, the approximate distance (all the way) to  $M_0$  is given by

$$\mathbb{D}_A^2(N_0, M_0) = \int_{\mathbb{T}_L^d} (N_0 |\nabla Q|^2 + \Omega_{N_0} Q^2) dx.$$

It is underscored, informally, that  $\mathbb{D}_A^2(N_0, M_0)$  – and  $Q$  – are of order unity relative to  $h$  with  $h \ll 1$ . We have (since the relevant equations are linear)

$$\mathbb{D}_A^2(N_0, M_\lambda^{(0)}) = h^2 \lambda^2 \mathbb{D}_A^2(N_0, M_0)$$

We now adjust  $\lambda$  so that this distance is exactly the distance which is traveled under the auspices of the JKO type process:

$$h^2 \lambda^2 \mathbb{D}_A^2(N_0, M_0) = \mathbb{D}_A^2(N_0, N_1).$$

Now since we must have  $\mathbb{J}_A(N_0, N_1) \leq \mathbb{J}_A(N_0, M_\lambda^{(0)})$ , it follows that  $\mathcal{G}_\mu(N_1) \leq \mathcal{G}_\mu(M_\lambda^{(0)})$ . Thus, using convexity of  $\mathcal{G}_\mu(\cdot)$  – which is legitimate since all densities are in  $\mathcal{B}_\kappa$  – we have

$$\mathcal{G}_\mu(N_1) - \mathcal{G}_\mu(M_0) \leq (1 - h\lambda)(\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)).$$

Thus, if we can get  $\lambda$  uniformly bounded below for an indefinite number of iterations of the process, the above would translate – in the standard notation – to

$$\mathcal{G}_\mu(N_{(k+1)h}^{[h]}) - \mathcal{G}_\mu(M_0) \leq (1 - h\lambda)(\mathcal{G}_\mu(N_{kh}^{[h]}) - \mathcal{G}_\mu(M_0)) \quad (31)$$

and thus in the  $h \rightarrow 0$  limit,  $\mathcal{G}_\mu(N_t) - \mathcal{G}_\mu(M_0) \leq e^{-\lambda t}[\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)]$ .

We turn our investigations to  $\lambda$ . Let us start with some preliminary estimates on  $\mathbb{D}_A^2(N_0, M_0)$ . We have

$$-\int_{\mathbb{T}_L^d} (M_0 - N_0)Q dx = \mathbb{D}_A^2(N_0, M_0) = \int_{\mathbb{T}_L^d} (N_0|\nabla Q|^2 + \Omega_{N_0}Q^2) dx. \quad (32)$$

So, using inequalities on both ends:

$$\|N_0 - M_0\|_{L^2} \cdot \|Q\|_{L^2} \geq \int_{\mathbb{T}_L^d} \Omega_{N_0}Q^2 dx. \quad (33)$$

It is now claimed that, pointwise,

$$\Omega_N \geq N^{\frac{1}{2}}. \quad (34)$$

Indeed, we write

$$\Omega_N = \frac{N^{\frac{1}{2}}}{\Phi_N} \left( N^{\frac{1}{2}}e^{-\frac{1}{2}(\mu - w_N)} - \frac{1}{N^{\frac{1}{2}}}e^{\frac{1}{2}(\mu - w_N)} \right) = N^{\frac{1}{2}} \frac{\sinh \frac{1}{2}\Phi_N}{\frac{1}{2}\Phi_N} \geq N^{\frac{1}{2}}.$$

Thus the bound in Eq.(33) may be replaced by

$$\|N_0 - M_0\|_{L^2} \cdot \|Q\|_{L^2} \geq (\kappa M_0)^{\frac{1}{2}} \|Q\|_{L^2}^2$$

i.e.,

$$\|Q\|_{L^2} \leq \frac{1}{(\kappa M_0)^{\frac{1}{2}}} \|N_0 - M_0\|_{L^2}.$$

Putting this back into Eq.(32) we acquire

$$\mathbb{D}_A^2(N_0, M_0) \leq \frac{1}{(\kappa M_0)^{\frac{1}{2}}} \|N_0 - M_0\|_{L^2}^2 := g^2 \|N_0 - M_0\|_{L^2}^2 \quad (35)$$

Since this implies

$$g^2 \|N_0 - M_0\|_{L^2}^2 h^2 \lambda^2 \geq \mathbb{D}_A^2(N_0, M_\lambda^{(0)}) = \mathbb{D}_A^2(N_0, N_1), \quad (36)$$

our goal will be achieved if we can show that  $\mathbb{D}_A^2(N_0, N_1)$  is of the same order as  $h^2 \|N_0 - M_0\|_{L^2}^2$ .

To this end, we will now consider

$$M_\theta^{(1)} := (1 - h\theta)N_1 + h\theta M_0.$$

The strategy here is to show that if  $\mathbb{D}_A^2(N_0, N_1)$  were not of the correct order of magnitude (according to the above stated goal) then  $M_\theta^{(1)}$  would be a better minimizer for  $\mathbb{J}_A(N_0, \cdot)$ . In what follows, let us use the version of  $\mathbb{J}_A$  in which the current value of the free energy is subtracted off:

$$\mathbb{J}_A(N_0, M_\theta^{(1)}) = \frac{1}{2}\mathbb{D}_A^2(N_0, M_\theta^{(1)}) + h(\mathcal{G}_\mu(M_\theta^{(1)}) - \mathcal{G}_\mu(N_0));$$

let us start with an upper bound on  $\mathbb{D}_A^2(N_0, M_\theta^{(1)})$ . To this end, it is noted that the driving field which achieves  $M_\theta^{(1)}$  is given by  $(1 - h\theta)\Phi_{N_1} + h\theta Q$ . Therefore

$$\mathbb{D}_A^2(N_0, M_\theta^{(1)}) = (1 - h\theta)^2\mathbb{D}_A^2(N_0, N_1) + h^2\theta^2\mathbb{D}_A^2(N_0, M_0) + 2h^2\theta(1 - h\theta)\langle\Phi_{N_1}, Q\rangle_{N_0}.$$

We will bound the last term by  $2h\theta(1 - h\theta)\mathbb{D}_A(N_0, N_1)\mathbb{D}_A(N_0, M_0)$  – note that these are not squared and one factor of  $h$  has been absorbed into the term  $\mathbb{D}_A(N_0, N_1)$ . I.e., we are using/deriving the (square of the) triangle inequality for the approximate distance. Meanwhile, by the convexity from Proposition 4.2,  $\mathcal{G}_\mu(M_\theta^{(1)}) \leq (1 - h\theta)\mathcal{G}_\mu(N_1) + h\theta\mathcal{G}_\mu(M_0)$ . Putting this together, we have

$$\begin{aligned} \mathbb{J}_A(N_0, M_\theta^{(1)}) &\leq \mathbb{J}_A(N_0, N_1) + h\theta\mathbb{D}_A(N_0, N_1)\mathbb{D}_A(N_0, M_0) + h^2\theta[\mathcal{G}_\mu(M_0) - \mathcal{G}_\mu(N_0)] \\ &\quad - h\theta[\mathbb{D}_A^2(N_0, N_1) + h(\mathcal{G}_\mu(N_1) - \mathcal{G}_\mu(N_0))] + \frac{1}{2}h^2\theta^2[\mathbb{D}_A(N_0, M_0) - \mathbb{D}_A(N_0, N_1)]^2 \end{aligned} \quad (37)$$

The right hand side must exceed  $\mathbb{J}_A(N_0, N_1)$  and so, subtracting this off, the remaining terms cannot be negative. In particular this is so when we divide by  $h\theta$  and take the  $\theta \rightarrow 0$  limit. Thus

$$h[\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)] \leq \mathbb{D}_A(N_0, N_1)\mathbb{D}_A(N_0, M_0) - [\mathbb{D}_A^2(N_0, N_1) + h(\mathcal{G}_\mu(N_1) - \mathcal{G}_\mu(N_0))]$$

Unfortunately, the term inside the brackets is in fact slightly negative – but manifestly of lower order in  $h$ . We will throw out the  $\mathbb{D}_A^2$ -term since it is positive and attend to the other term later. The principal task at hand is the following:

**Claim** Under the conditions on  $M_0$  and  $\kappa$  in the statement of this theorem, there is a  $\sigma = \sigma(M_0, \kappa) > 0$  such that

$$\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0) \geq \sigma\|N_0 - M_0\|_{L^2}^2.$$

*Proof of Claim.* This, it turns out, is a recapitulation of (the convexity) Proposition 4.2. If we write  $N_0 = M_0 + (N_0 - M_0)$  we can expand the free energy in powers of  $N_0 - M_0$ . The first order term vanishes by stationarity while the interaction piece is exact at the quadratic order. Now, pointwise,

$$[M_0 + (N_0 - M_0)] \log[M_0 + (N_0 - M_0)] = M_0 \log M_0 + \text{linear piece} + \frac{1}{2} \frac{[N_0 - M_0]^2}{\nu N_0 + (1 - \nu)M_0}$$

where  $\nu \in [0, 1]$  depends on the value of  $N_0(x)$ . Thus we may write

$$\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0) = \frac{1}{2} \int_{\mathbb{T}_L^d} \frac{R_0^2 dx}{\nu(x)N_0 + (1 - \nu(x))M_0} + \frac{1}{2} \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)R_0(x)R_0(y)dx dy$$

with  $R_0(x)$  temporary notation for  $N_0(x) - M_0$ . The conclusion follows with

$$\sigma = \frac{1}{2} \left( \frac{\kappa}{M_0} - \frac{1}{\vartheta^\sharp} \right).$$

The stated claim has been established.  $\blacksquare$

Thus, the equation just prior to the statement of the above claim can be combined with Eq.(35) so we get

$$h\sigma \|N_0 - M_0\|_{L^2}^2 + h(\mathcal{G}_\mu(N_1) - \mathcal{G}_\mu(N_0)) \leq g\mathbb{D}_A(N_0, N_1) \|N_0 - M_0\|_{L^2} \quad (38)$$

and, were it not for the hindrance of the small term,  $h(\mathcal{G}_\mu(N_1) - \mathcal{G}_\mu(N_0))$ , on the left, we would obtain a lower bound of  $\frac{h\sigma}{g} \|N_0 - M_0\|_{L^2}$  for  $\mathbb{D}_A(N_0, N_1)$  which would imply

$$\lambda \geq \frac{\sigma}{g^2} := \lambda^\dagger.$$

Unfortunately, the small free energy difference term will appear at each stage of the iteration and there are of order  $h^{-1}$  steps altogether. To handle this matter, let us take the time to write Eq.(38) in the form that it would appear without the abbreviations:

$$h\sigma \|N_{kh}^{[h]} - M_0\|_{L^2}^2 + h \left( \mathcal{G}_\mu(N_{(k+1)h}^{[h]}) - \mathcal{G}_\mu(N_{kh}^{[h]}) \right) \leq g\mathbb{D}_A \left( N_{kh}^{[h]}, N_{(k+1)h}^{[h]} \right) \|N_{kh}^{[h]} - M_0\|_{L^2}.$$

Let us stipulate that, necessarily, for all times  $t' < t$ ,  $N_{t'} \neq M_0$  (indeed, otherwise there would be nothing to prove). Thus, it is clear that

$$\epsilon := \inf_{k, h: h k \leq t} \|N_{kh}^{[h]} - M_0\|_{L^2}^2$$

is strictly positive. We shall only consider  $h$ 's which satisfy  $h < \epsilon^2$  and thus the above generalization of Eq.(38) in combination with Eq.(36) yields the estimate

$$h\lambda_{k+1} \geq \frac{\mathbb{D}_A(N_{hk}^{[h]}, N_{h(k+1)}^{[h]})}{g\|N_{hk}^{[h]} - M_0\|_{L^2}} \geq \left[ \frac{h\sigma}{g^2} + \frac{h^{\frac{1}{2}}}{g^2} \left( \mathcal{G}_\mu(N_{h(k+1)}^{[h]}) - \mathcal{G}_\mu(N_{hk}^{[h]}) \right) \right].$$

Recalling the discussion surrounding the display labeled (31) we now have the estimate

$$\mathcal{G}_\mu(N_{(k+1)h}^{[h]}) - \mathcal{G}_\mu(M_0) \leq [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)] \prod_{j=1}^k (1 - h\lambda_j).$$

We bound the product:

$$\begin{aligned} \prod_{j=1}^k (1 - h\lambda_j) &= (1 - h\lambda^\dagger)^k \prod_{j=1}^k \left( 1 - \frac{h^{\frac{1}{2}}}{g(1 - h\lambda^\dagger)} \left( \mathcal{G}_\mu(N_{h(k+1)}^{[h]}) - \mathcal{G}_\mu(N_{hk}^{[h]}) \right) \right) \\ &\leq (1 - h\lambda^\dagger)^k \text{Exp} \left[ -\frac{h^{\frac{1}{2}}}{g(1 - h\lambda^\dagger)} \sum_{j=1}^k \left( \mathcal{G}_\mu(N_{h(k+1)}^{[h]}) - \mathcal{G}_\mu(N_{hk}^{[h]}) \right) \right]. \quad (39) \end{aligned}$$

The sum in the exponent is just the current free energy drop which may be bounded uniformly in  $k$  by the total free energy drop, namely  $\mathcal{G}_\mu(M_0) - \mathcal{G}_\mu(N_0)$ , and the pre-factor of  $h^{\frac{1}{2}}$  causes this factor in the exponent to vanish in the  $h \rightarrow 0$  limit. Thus, as claimed, when we take  $h \rightarrow 0$

$$\mathcal{G}_\mu(N_t) - \mathcal{G}_\mu(M_0) \leq [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)]e^{-\lambda^\dagger t}$$

By the result displayed in the above claim, a similar estimate holds for  $\|N_t - M_0\|_{L^2}^2$ .  $\square$

Finally, we claim that in essence, the derivation featured starting at Eq.(32) and ending at Eq.(35) also holds for the *actual*  $\mathbb{D}$ -distance:

**Corollary 4.4** *With all notation as before, we have*

$$\mathbb{D}^2(N_t, M_0) \leq \frac{g^2}{\sigma} [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)]e^{-\lambda^\dagger t}.$$

*Proof.* Let  $N \in \mathcal{B}_\kappa$  and consider

$$N_s^\bullet = (1 - s)N + sM_0.$$

Let  $Q_s^\bullet$  denote the corresponding advective potential

$$\frac{\partial N_s^\bullet}{\partial s} \equiv M_0 - N = \nabla \cdot (N_s^\bullet \nabla Q_s^\bullet) - \Omega_{N_s^\bullet} Q_s^\bullet.$$

Obviously  $Q_s^\bullet$  depends on  $s$ . Now going this route from  $N \rightarrow M_0$  will not necessarily minimize the actual distance functional:

$$\mathbb{D}^2(N, M_0) \leq \int_0^1 \langle \nabla Q_s^\bullet, \nabla Q_s^\bullet \rangle_{N_s^\bullet} ds$$

so an upper bound on the integrated inner product constitutes an upper bound on the actual distance.

But the above mentioned derivation also works on this inner product:

$$\begin{aligned} \|M_0 - N\|_{L^2} \left( \int_0^1 \|Q_s^\bullet\|_{L^2}^2 ds \right)^{\frac{1}{2}} &\geq - \int_0^1 ds \int_{\mathbb{T}_L^d} (M_0 - N) Q_s^\bullet dx \\ &= \int_0^1 \langle \nabla Q_s^\bullet, \nabla Q_s^\bullet \rangle_{N_s^\bullet} ds \geq \frac{1}{2} (\kappa M_0)^{\frac{1}{2}} \int_0^1 \|Q_s^\bullet\|_{L^2}^2 ds \end{aligned} \quad (40)$$

and we arrive at the same bound as in Eq.(35).

Thence we may conclude

$$\mathbb{D}^2(N_t, M_0) \leq \frac{g^2}{\sigma} [\mathcal{G}_\mu(N_0) - \mathcal{G}_\mu(M_0)]e^{-\lambda^\dagger t}.$$

$\square$

*Proof of Theorem 1.2.* The establishment of  $\mathbb{D}(\cdot, \cdot)$  as a *bona fide* distance is found in Appendix B and the convergence of the JKO type scheme is the content of Theorem 3.8. Finally, Corollary 4.4 establishes the stated convergence for the distance  $\mathbb{D}(\cdot, \cdot)$ .

## 5 Appendix A

In this appendix, we analyze the discrete time evolution of the fluid density as given in Eq.(22). While this equation produces  $N_{(k+1)h}$  from  $N_{kh}$  in order to avoid clutter, we will set  $k = 0$  – and introduce various other abbreviations to be described shortly. The ultimate result depends only on properties of  $N_k$  (AKA  $N_0$ ) primarily a  $\mathcal{D}_2$ –norm (a Fourier norm) described below. Thus, the principal difficulty will be to show that the relevant properties are preserved under iteration. And, it turns out, it is too much to expect that this is achieved by having the incremental changes in e.g.,  $N_0$ ,  $\nabla^2 N_0$  etc., to always be of order  $h$ . Thus a somewhat delicate (albeit presumably standard) “cancelation” must be exhibited in the course of our arguments.

### 5.1 The Full Equation

Equation (22) is most conveniently expressed in terms of the variable  $\Psi := \log N$ . For the purposes of this appendix, we will abbreviate  $\Psi_0 := \log N_0$  and  $w_0 := W * N_0$  with similar notational conventions when 0–subscripts are replaced by 1’s. In this language, Eq.(22) reads

$$e^{\Psi_1 - \Psi_0} - 1 = h[\nabla^2 \Psi_1 + \nabla^2 w_1 + \nabla \Psi_1 \cdot \nabla \Psi_0 + \nabla w_1 \cdot \nabla \Psi_0] - h(\Psi_1 + w_1)e^{-\Psi_0}\Omega_{N_0}. \quad (41)$$

Introducing  $h\psi := \Psi_1 - \Psi_0$ , Eq.(41) now reads

$$\begin{aligned} \frac{e^{h\psi} - 1}{h} = & h\nabla^2 \psi + [\nabla^2 \Psi_0 + |\nabla \Psi_0|^2 + \nabla^2 w_0 + \nabla w_0 \cdot \nabla \Psi_0 - (\Psi_0 + w_0)\Omega_0] \\ & + h[\nabla^2 w_\psi + \nabla w_\psi \cdot \nabla \Psi_0 + \nabla \psi \cdot \nabla \Psi_0 - \psi\Omega_0 - w_\psi\Omega_0] \end{aligned} \quad (42)$$

where we have further used the abbreviations  $\Omega_0$  which is given by  $\Omega_0 := e^{-\Psi_0}\Omega_{N_0}$  and  $w_\psi$  defined by  $hw_\psi := w_1 - w_0 = W * (e^{\Psi_0})(e^{h\psi} - 1)$ .

The advantage of using the  $\Psi$ –variables is now manifest: all of the non–linearities of this equation are encoded into the function itself and do not involve the derivatives.

### 5.2 Norms

Our analyses will be essentially classical – although it is conceivable that with greater effort, a more general treatment would be possible. In any case we will start with an assumption on  $\Psi_0$  – which is slightly stronger than  $H^1$  – in particular we will require that  $\Psi_0 \in \mathcal{D}_2$  as described below:

Let  $f : \mathbb{T}_L^d \rightarrow \mathbb{R}$  have Fourier coefficients  $\hat{f}(k)$ . Then

$$\|f\|_{\mathcal{D}_0} := \frac{1}{L^d} \sum_k |\hat{f}(k)|$$



and, if this is finite, we say  $f \in \mathcal{D}_0$ . In general,

$$\|f\|_{\mathcal{D}_m} := \frac{1}{L^d} \sum_k |k|^m |\hat{f}(k)|$$

defines the class  $\mathcal{D}_m$ . It is noted that these norms obey the usual inequalities e.g.,  $\|f\|_{\mathcal{D}_1}^2 \leq \|f\|_{\mathcal{D}_2} \|f\|_{\mathcal{D}_0}$  and have derivation properties e.g.,  $\|fg\|_{\mathcal{D}_1} \leq \|f\|_{\mathcal{D}_1} \|g\|_{\mathcal{D}_0} + \|f\|_{\mathcal{D}_0} \|g\|_{\mathcal{D}_1}$ .

Our precise assumption is that  $\Psi_0 \in \mathcal{D}_2$  with a bound on the norm that does not depend on  $h$ . The latter is emphasized because, e.g., for the time interval  $[0, T]$ , we must accommodate the order of  $Th^{-1}$  iterations of Eq.(22). Of course a single application is readily accomplished with the result  $\Psi_1 \sim \Psi_0 + h[\nabla^2 \Psi_0 + |\nabla \Psi_0|^2 + \dots - w_0 \Omega_0]$ . But this perturbative result, in and of itself, cannot be expected to get us through too many iterations. For us, among other small matters, the crucial requirement is to show that the actual  $\Psi_1$  also has a  $\mathcal{D}_2$ -norm which is uniformly bounded independent of  $h$  – provided that  $h$  is sufficiently small – in order that the above heuristic can be continued.

The above notions will be placed on a more formal footing. Let us amalgamate into a set – denoted by  $\mathfrak{D}$  – all the relevant input constants:

$$\mathfrak{D} = \{\|\Psi_0\|_{\mathcal{D}_0}, \|\Psi_0\|_{\mathcal{D}_2}, v_0, \dots, v_4, \|W\|_{\mathcal{D}^2}\}$$

where the  $v_m$  are given by  $v_m := \sup_k |\hat{W}(k)| |k|^m$  and are assumed to be finite for  $m \leq 4$ . These are regarded as *fixed* while the time step parameter is to be treated as a variable, albeit “small”. In the course of our analysis, various numbers will emerge which will depend on  $\mathfrak{D}$  but not on  $h$ . Then, these numbers are bounded provided the elements of  $\mathfrak{D}$  are bounded. The time-step  $h$  itself will be allowed to take on any value smaller than some  $h_0$  which, ultimately, *does* depend on  $\mathfrak{D}$ . But, again,  $h_0$  will be bounded (below) provided the elements of  $\mathfrak{D}$  are bounded (above). These numbers provide us with the updated version of  $\mathfrak{D}$  which (if all goes according to plan) will also have elements which have only incremented by the order of  $h$  and thus, at least for a while, may be regarded as bounded independently of  $h$ . Thence, the whole process can be continued throughout some finite interval  $[0, T]$  – the order of  $h^{-1}T$  iterations – with bounds that will depend only on the initial condition and, perhaps,  $T$ .

Of course only two of the elements of  $\mathfrak{D}$  are destined to change; later these will be referred to as the *mutable* elements. Anticipated but conspicuously absent from the mutable elements of  $\mathfrak{D}$  is the quantity  $\|\Psi_0\|_{\mathcal{D}_1}$ . The reason is economical rather than esoteric: Below begins the  $\mathcal{D}_0$ -analysis followed in Subsection 5.4 by the  $\mathcal{D}_2$ -analysis which is still more substantial. In principal, a  $\mathcal{D}_1$  subsection could have been written which, presumably, would have been intermediate. In practice, we are (at first) interested in bounds which permit iteration of the process for *some* positive

macroscopic time. Therefore it proves to be sufficient, even if less efficient, to use  $||\Psi_0||_{\mathcal{D}_2}^{\frac{1}{2}} ||\Psi_0||_{\mathcal{D}_0}^{\frac{1}{2}}$  as an upper bound for  $||\Psi_0||_{\mathcal{D}_1}$  in the places where such a bound on this quantity is required.

### 5.3 Preliminary Analysis

We start off with a bound on the  $\mathcal{D}_0$ -norm of  $\psi$ :

**Proposition 5.1** *There is an  $h_2$  such that for all  $h \leq h_2$ , we have  $||\psi||_{\mathcal{D}_0} \leq \mathfrak{b}_0$ ; both  $\mathfrak{b}_0$  and  $h_2$  depend only on  $\mathfrak{D}$  and are uniformly bounded for bounded ranges of these elements.*

*Proof.* We start with a rewrite of Eq.(42) so that it takes the form

$$\psi - h\nabla^2 \psi = A + hB_\psi - \frac{1}{h}\mathcal{E}_2(h\psi) \quad (43)$$

where in the above  $\mathcal{E}_2(x) = \sum_{m \geq 2} \frac{x^m}{m!}$  (and, for future reference, similarly for  $\mathcal{E}_1$ ) and the  $A$  and  $B_\psi$  correspond to the appropriate bracketed terms in the above mentioned equation – so that in particular the  $A$  term is entirely determined by  $\mathfrak{D}$ . Thus we may write

$$\psi = \underline{L}_h^{-1}(A + hB_\psi - \frac{1}{h}\mathcal{E}_2(h\psi)) \quad (44)$$

where  $\underline{L}_h := 1 - h\nabla^2$ . We estimate the terms one at a time adding all the results; most terms are handled easily with the neglect of  $\underline{L}_h^{-1}$ . E.g.,

$$||\underline{L}_h^{-1}(\nabla^2 \Psi_0)||_{\mathcal{D}_0} = \frac{1}{L^d} \sum_k \frac{1}{1 + hk^2} \cdot k^2 |\hat{\Psi}_0| \leq \frac{1}{L^d} \sum_k k^2 |\hat{\Psi}_0| = ||\Psi_0||_{\mathcal{D}_2}.$$

As a further illustration we bound  $||\underline{L}_h^{-1} \nabla^2 w_0||_{\mathcal{D}_0} \leq ||w_0||_{\mathcal{D}_2} \leq v_2 ||e^{\Psi_0}||_{\mathcal{D}_0} \leq v_2 e^{||\Psi_0||_{\mathcal{D}_0}}$ . All terms in  $A$  can be handled this way.

The  $B_\psi$ -terms as well as the final term now involve  $\psi$  itself. Nevertheless, most of the *bounds* are completely straightforward. E.g.,  $\frac{1}{h} ||\underline{L}_h^{-1} \mathcal{E}_2(h\psi)||_{\mathcal{D}_0} \leq \frac{1}{h} \mathcal{E}_2(h||\psi||_0)$  and similarly for all of the  $B_\psi$ -terms save for the third. For the third we use

$$\begin{aligned} ||h\underline{L}_h^{-1}(\nabla\psi \cdot \nabla\Psi_0)||_{\mathcal{D}_0} &\leq \frac{1}{L^{2d}} \sum_{k,q} \left| \frac{h}{1+hk^2} (k-q) \cdot q \hat{\Psi}_0(q) \hat{\psi}(k-q) \right| \\ &\leq h||\psi||_{\mathcal{D}_0} ||\Psi_0||_{\mathcal{D}_2} + \frac{1}{L^{2d}} \sum_{k,q} \frac{h|k|}{1+hk^2} |\hat{\psi}(k-q)| |q| |\Psi_0(q)|. \end{aligned} \quad (45)$$

To handle the the final term in Eq.(45) above, we use  $\frac{h|k|}{1+hk^2} \leq \frac{1}{2}h^{\frac{1}{2}}$  and this quantity is bounded by  $\frac{1}{2}h^{\frac{1}{2}} ||\psi||_{\mathcal{D}_0} ||\Psi_0||_{\mathcal{D}_1}$ .

The “bound” now takes the form

$$||\psi||_{\mathcal{D}_0} \leq A_0 + b_0 h^{\frac{1}{2}} ||\psi||_{\mathcal{D}_0} + h\beta_0 ||\psi||_{\mathcal{D}_0} + hG(h, ||\psi||_{\mathcal{D}_0}) \quad (46)$$

where all constants and functions depend (uniformly) only on the parameters in  $\mathfrak{D}$  and the quantity  $G$  tends down to another such constant as  $h \rightarrow 0$ ; importantly,  $\|\psi\|_{\mathcal{D}_1}$  does *not* appear in the estimate. Thus, we may tentatively conclude that  $\|\psi\|_{\mathcal{D}_0} \lesssim A_0$ . However, it is noted that given the form of the right hand side of the above display, there is also the possible interpretation of a trivial (i.e., infinite) bound; an issue we now address.

Let us denote the right side by  $\Xi(h, \|\psi\|_{\mathcal{D}_0})$ ; so we write  $\|\psi\|_{\mathcal{D}_0} \leq \Xi(h, \|\psi\|_{\mathcal{D}_0})$ . First, let us examine the recursive equation

$$\zeta_{k+1} = \Xi(h, \zeta_k) \quad (47)$$

with  $\zeta_0 = A_0$ . It is noted, by monotonicity/convexity properties of  $\Xi$  (in the variable  $\zeta$ ) that there is an  $h_1$  such that for  $h < h_1$  there is a  $\zeta_\# = \zeta_\#(h)$  which is the unique stable fixed point of Eq.(47) so that if  $\zeta_j < \zeta_\#$  then  $\zeta_j < \zeta_{j+1} < \zeta_\#$  and  $\lim_{j \rightarrow \infty} \zeta_j = \zeta_\#$ . (Moreover, necessarily,  $\zeta_0 < \zeta_\#$ .)

Thus, starting with  $\psi_0 = \underline{L}_h^{-1}(A)$  we may define  $\psi_{j+1}$  via the right hand side of Eq.(43) acting on (or, as a function of)  $\psi_j$ . This guarantees  $\|\psi_j\|_{\mathcal{D}_0} \leq \zeta_j < \zeta_\#$ . Let  $\psi$  be a weak limit of the  $\psi_j$ 's. It remains to identify  $\psi$  with the object featured in Eq.(43).

To this end we consider  $\delta_j := \psi_j - \psi_{j-1}$ . When we compute this quantity, much of the old  $\Xi$  survives and we arrive at

$$\|\delta_j\|_{\mathcal{D}_0} \leq h^{\frac{1}{2}} \|\delta_j\|_{\mathcal{D}_0} \Gamma(h, \|\delta_j\|_{\mathcal{D}_0}, \|\psi_{j-1}\|_{\mathcal{D}_0}).$$

For example, a contribution to  $\Gamma$ :

$$\begin{aligned} \frac{1}{h} \|\mathcal{E}_2(h\psi_j) - \mathcal{E}_2(h\psi_{j-1})\|_{\mathcal{D}_0} &= \left\| \frac{1}{h} e^{h\psi_{j-1}} \mathcal{E}_2(h\delta_j) + \delta_j \mathcal{E}_1(h\psi_{j-1}) \right\|_{\mathcal{D}_0} \\ &\leq \frac{1}{h} e^{h\|\psi_{j-1}\|_{\mathcal{D}_0}} \mathcal{E}_2(h\|\delta_j\|_{\mathcal{D}_0}) + \delta_j \mathcal{E}_1(h\|\psi_{j-1}\|_{\mathcal{D}_0}). \end{aligned}$$

The properties of  $\Gamma$  are manifest, e.g., it tends to a definitive constant as  $h \downarrow 0$  and is uniformly bounded provided its arguments are.

Consider  $\zeta_{\#\#}$  which is the limit as  $h \rightarrow h_1$  of  $\zeta_\#(h)$ . Let  $h_2$  be defined by

$$[h_2]^{\frac{1}{2}} \times \left[ \sup_{\substack{h < h_1 \\ b < \zeta_{\#\#}, a < 2\zeta_{\#\#}}} \Gamma(h, a, b) \right] = 1.$$

The conclusion is clear: For  $h < h_2$ ,  $\psi_j$  converges (strongly in  $\mathcal{D}_0$ ) to the  $\psi$  given in Eq.(44) and for  $h < h_2$  we have  $\forall j$  the  $\psi_j$ 's and the limiting  $\psi$  bounded in  $\mathcal{D}_0$  by  $\zeta_\#(h_2)$ . Moreover, all parameters,  $h_1, h_2 \dots \zeta_\#(h_2)$  depend only on the parameters of  $\mathfrak{D}$  and are uniformly in accord with the range of these elements.  $\square$

## 5.4 Advanced Analysis

The situation concerning the  $\mathcal{D}_2$ -norm of  $\psi$  will not be as straightforward as that of the above – indeed, there is no hope for a result analogous to Proposition 5.1. In particular, let us investigate the very first term

$$\psi_\star := \underline{L}_h^{-1}(\nabla^2 \Psi_0) \quad (48)$$

While it is clear that  $\|\psi_\star\|_{\mathcal{D}_2} < \infty$ , this norm might well be divergent as  $h \downarrow 0$ ; e.g.,  $\|h\psi_\star\|_{\mathcal{D}_2}$  could be a sublinear power of  $h$ . However, as will be demonstrated, this is actually beneficial: in a certain sense, the more divergent the better. Indeed, let us define the “preliminary correction”

$$\Psi_\star := \Psi_0 + h\psi_\star.$$

Then

$$\hat{\Psi}_\star(k) = \hat{\Psi}_0(k) - \frac{hk^2}{1+hk^2} \hat{\Psi}_0(k) = \frac{\hat{\Psi}_0(k)}{1+hk^2}. \quad (49)$$

i.e., the magnitude of *every* non-zero mode has been reduced. Hence, the task at hand will be to show that the rest of  $\psi$  does not disrupt these benefits. Specifically, defining

$$\psi_\bullet := \psi - \psi_\star$$

our aim is to show that the difference,  $\|\psi_\bullet\|_{\mathcal{D}_2} - \|\psi_\star\|_{\mathcal{D}_2}$ , is either negative or of order unity.

We remark that in contrast to the preceding analysis, there is no reason to expect matching with powers of  $h$ . Thus, we will be working directly with  $h\psi_\star$ ,  $h\psi_\bullet$ , etc., even though, at times, appearances of  $h$ , e.g., multiplying both sides of an equation, may seem redundant.

The preliminary challenge arises from the ranks of the inhomogeneous terms. We define  $r_\bullet$  and  $s_\bullet$  via:

$$hr_\bullet := h\underline{L}_h^{-1}(|\nabla \Psi_0|^2) \quad \text{and} \quad hs_\bullet := h\underline{L}_h^{-1}(\nabla \Psi_0 \cdot \nabla w_0).$$

Our first goal is an estimate on their  $\mathcal{D}_2$  norms. We start by invoking the relevant length scale for these problems:

**Definition 5.2.** Let  $p_0 = p_0(h)$  be such that

$$\frac{1}{L^d} \sum_{p:|p| \geq p_0} |p \hat{\Psi}_0(p)| \geq h$$

while without the last shell,

$$\frac{1}{L^d} \sum_{p:|p| > p_0} |p \hat{\Psi}_0(p)| < h.$$

**Claim A<sub>1</sub>.** There is an  $a$  depending only on  $\mathfrak{D}$  such that if  $p_0 > ah^{-\frac{1}{2}}$  then

$$||h\psi_\star||_{\mathcal{D}_2} \geq 2[||hr_\bullet||_{\mathcal{D}_2} + ||hs_\bullet||_{\mathcal{D}_2}].$$

*Proof of Claim.* We first note that, *a priori*,  $||hr_\bullet||_{\mathcal{D}_2}$  and  $||hs_\bullet||_{\mathcal{D}_2}$  do not exceed the order of  $h^{\frac{1}{2}}$ . Indeed, we write

$$hk^2\hat{r}_\bullet(k) = -\frac{hk^2}{1+hk^2} \frac{1}{L^{2d}} \sum_q \hat{\Psi}_0(q)q \cdot (k-q)\hat{\Psi}_0(k-q) \quad (50)$$

so, taking absolute values etc., and bringing one factor of  $k$  inside the sum,

$$|hk^2\hat{r}_\bullet(k)| \leq \frac{h|k|}{1+hk^2} \frac{1}{L^{2d}} \sum_q (q^2|k-q| + (k-q)^2|q|)|\Psi_0(q)||\Psi_0(k-q)|.$$

Using  $h^{\frac{1}{2}}|k|/(1+hk^2) \leq \frac{1}{2}$ , and summing over  $k$ , we are left with  $\frac{1}{2} \times 2 \times ||\Psi_0||_{\mathcal{D}_1} ||\Psi_0||_{\mathcal{D}_2}$ :

$$||hr_\bullet||_{\mathcal{D}_2} \leq h^{\frac{1}{2}} ||\Psi_0||_{\mathcal{D}_1} ||\Psi_0||_{\mathcal{D}_2}.$$

Similarly,

$$||hs_\bullet||_{\mathcal{D}_2} \leq \frac{1}{2} h^{\frac{1}{2}} [||\Psi_0||_{\mathcal{D}_2} ||w_0||_{\mathcal{D}_1} + ||\Psi_0||_{\mathcal{D}_1} ||w_0||_{\mathcal{D}_2}]$$

On the other hand,

$$||h\psi_\star||_{\mathcal{D}_2} \geq \frac{1}{L^d} \sum_{k:|k| \geq p_0} \frac{hk^2}{1+hk^2} \cdot k^2 |\hat{\Psi}_0(k)| \geq \frac{hp_0^3}{1+hp_0^2} \frac{1}{L^d} \sum_{k:|k| \geq p_0} |k| |\hat{\Psi}_0(k)| \geq \frac{h^2 p_0^3}{1+hp_0^2}$$

Thus, if  $p_0 \geq ah^{-\frac{1}{2}}$  where  $a$  is given by

$$\frac{a^3}{1+a^2} = 2[||\Psi_0||_{\mathcal{D}_2} ||w_0||_{\mathcal{D}_1} + \frac{1}{2} (||\Psi_0||_{\mathcal{D}_2} ||w_0||_{\mathcal{D}_1} + ||\Psi_0||_{\mathcal{D}_1} ||w_0||_{\mathcal{D}_2})]$$

the claim is established.  $\blacksquare$

We may proceed under the assumption that  $p_0 < ah^{-\frac{1}{2}}$  since otherwise, the  $r_\bullet$  and  $s_\bullet$  terms are well in hand.

**Claim A<sub>2</sub>.** Our next claim is that, under the assumption  $p_0 < ah^{-\frac{1}{2}}$  both  $r_\bullet$  and  $s_\bullet$  admit the bounds

$$\begin{aligned} ||hr_\bullet||_{\mathcal{D}_2} &\leq C_r ||h\underline{L}_h^{-1} \Psi_0||_{\mathcal{D}_3} + hc_r \\ ||hs_\bullet||_{\mathcal{D}_2} &\leq C_s ||h\underline{L}_h^{-1} \Psi_0||_{\mathcal{D}_3} + hc_s \end{aligned} \quad (51)$$

where  $C_r, \dots, c_s$  are constants which depend only on  $\mathfrak{D}$

*Proof of Claim.* Let us proceed with the analysis of Eq.(50) taking absolute values etc., and summing over  $k$  at fixed  $q$ . First, we investigate the region where  $|k-q| > p_0$ . Here we may use  $hk^2/[1+hk^2] < 1$  leaving us with

$$\frac{1}{L^d} |q| |\hat{\Psi}_0(q)| \frac{1}{L^d} \sum_{k:|k-q| > p_0} |k-q| |\hat{\Psi}_0(k-q)| \leq h \frac{1}{L^d} |q| |\hat{\Psi}_0(q)|.$$

The summation over  $q$  gives the bound  $h\|\Psi_0\|_{\mathcal{D}_1}$  which is part of the  $c_r$ -term. What remains to be estimated is the quantity

$$\frac{1}{L^{2d}} \sum_{k,q:|k-q|\leq p_0} \frac{hk^2}{1+hk^2} |q| |\hat{\Psi}_0(q)| |k-q| |\hat{\Psi}_0(k-q)|.$$

Similarly to the above, if we first allow summation over  $q$  with  $|q| > p_0$  we may divest of the factor  $hk^2/(1+hk^2)$  and, now summing over  $q$  with  $(k-q)$  fixed – and even unrestricted – after the summation over  $q$  and  $k-q$ , we arrive at another estimate of  $h\|\Psi_0\|_{\mathcal{D}_1}$  which we add to the  $c_r$ -term.

Thus, for all intents and purposes we may restrict to  $|q|, |k-q| < p_0$ . Here, for the  $k^2$  in the numerator we write  $k^2 = q^2 + (k-q)^2 + 2q \cdot (k-q)$  giving us three terms to estimate the first of which is

$$\frac{1}{L^{2d}} \sum_{k,q:|q|,|k-q|\leq p_0} \frac{h}{1+hk^2} |q|^3 |\hat{\Psi}_0(q)| |k-q| |\hat{\Psi}_0(k-q)|$$

Now  $\frac{1}{1+hk^2} < 1$  and also  $1+hq^2 \leq 1+a^2$  so the upshot is that the above term is bounded above by

$$h(1+a^2) \frac{1}{L^{2d}} \sum_{k,q} \frac{1}{1+hq^2} |q|^3 |\hat{\Psi}_0(q)| |k-q| |\hat{\Psi}_0(k-q)|$$

where we have now relaxed the restriction on the range of summation. Summing over  $k$  we acquire our first contribution to  $C_r$ , namely  $(1+a^2)\|\Psi_0\|_{\mathcal{D}_1}$ .

The second term is the quantity

$$\frac{2}{L^{2d}} \sum_{k,q:|q|,|k-q|\leq p_0} \frac{h}{1+hk^2} q^2 |\hat{\Psi}_0(q)| (k-q)^2 |\hat{\Psi}_0(k-q)|,$$

we relax the restriction over the summation and use  $[1+hk^2]^{-1} < 1$  to arrive at the bound of  $2h\|\Psi_0\|_{\mathcal{D}_2}^2$  which is another contribution to the  $c_r$ -term. Our third term is identical to the first with the roles of  $q$  and  $k-q$  switched and may be estimated by the identical procedure.

The analysis of  $s_\bullet$  follows a similar set of procedures. We will dispense with the details and state the result:

$$C_s = (1+a^2)\|w_0\|_{\mathcal{D}_1}$$

and

$$c_s = \|w_0\|_{\mathcal{D}_1} + 2\|\Psi_0\|_{\mathcal{D}_2}\|w_0\|_{\mathcal{D}_2} + \|\Psi_0\|_{\mathcal{D}_1}\|w_0\|_{\mathcal{D}_3}.$$

The claim is established.  $\blacksquare$

Thus so far – on the basis that  $p_0 \leq ah^{-\frac{1}{2}}$  – we now have the  $r_\bullet$  and  $s_\bullet$  – terms essentially bounded by  $\|h\underline{L}_h^{-1}\Psi_0\|_{\mathcal{D}_3}$ . The next step is the following:

**Claim A<sub>3</sub>.** Either

$$||h\psi_\star||_{\mathcal{D}_2} > (C_r + C_s)||hL_h^{-1}\Psi_0||_{\mathcal{D}_3}$$

(where the difference may be considerable) or both  $||\psi_\star||_{\mathcal{D}_2}$  and  $||L_h^{-1}\Psi_0||_{\mathcal{D}_3}$  are bounded above by constants depending only on  $\mathfrak{D}$ .

*Proof of Claim.* We compare term by term:

$$\frac{|q^4|}{1+hq^2}|\hat{\Psi}_0(q)| \quad \text{vs.} \quad (C_r + C_s)\frac{|q^3|}{1+hq^2}|\hat{\Psi}_0(q)|;$$

obviously if  $|q| \geq (C_r + C_s)$  the terms contributing to  $||\psi_\star||_{\mathcal{D}_2}$  are dominant. Let us define  $q_0 := 2(C_r + C_s)$  and write  $||\psi_\star||_{\mathcal{D}_2} = \underline{a} + b$  where

$$\underline{a} = \sum_{|q| \leq q_0} \frac{q^4}{1+hq^2}|\hat{\Psi}_0(q)|, \quad b = \sum_{|q| > q_0} \frac{q^4}{1+hq^2}|\hat{\Psi}_0(q)|$$

and a similar decomposition ( $|q| \leq q_0$ ,  $|q| > q_0$ ) for  $(C_r + C_s)||\underline{L}_h^{-1}\Psi_0||_{\mathcal{D}_3}$  denoted by  $\underline{\alpha}$  and  $\beta$ . So, let us suppose  $\underline{a} + b \leq \underline{\alpha} + \beta$ . Since we have arranged  $b \geq 2\beta$  this implies  $\underline{a} \leq \underline{\alpha} - \beta$  hence  $\underline{a} \geq \beta$  and so

$$||\psi_\star||_{\mathcal{D}_2} \leq 2\underline{\alpha} = 2(C_r + C_s) \sum_{|q| \leq q_0} \frac{|q|^3}{1+hq^2}|\hat{\Psi}(q)| \leq q_0^2||\Psi_0||_{\mathcal{D}_2}.$$

I.e.,  $||h\psi_\star||_{\mathcal{D}_2}$  is actually of order  $h$ . The same bound (and conclusion) holds for  $||\underline{L}_h^{-1}\Psi_0||_{\mathcal{D}_3}$  which – also – does not exceed  $2\underline{\alpha}$ .  $\blacksquare$

**Proposition 5.3** *The  $\mathcal{D}_2$ -norms of  $\Psi_0$  and its successor  $\Psi_1$ , acquired after one iteration of the discretization, satisfy*

$$||\Psi_1||_{\mathcal{D}_2} - ||\Psi_0||_{\mathcal{D}_2} \leq \mathfrak{b}_2 h$$

where  $\mathfrak{b}_2$  depends only on the elements of  $\mathfrak{D}$ .

We reiterate that the left hand side in the above display can be considerably negative.

*Proof.* As discussed earlier, the proof of the proposition amounts to the same statement about  $||h\psi_\bullet||_{\mathcal{D}_2} - ||h\psi_\star||_{\mathcal{D}_2}$ . There are three terms in the expression for  $h\psi_\bullet$  which must be dealt with explicitly: These are the  $r_\bullet$  and  $s_\bullet$ -terms as well as the term  $h^2\nabla\psi \cdot \nabla\Psi_0$ . All other terms can be handled with straightforward methods. We shall be content with a couple of examples:

$$||h\underline{L}_h^{-1}(\nabla^2 w_0)||_{\mathcal{D}_2} = \frac{1}{L^d} \sum_k \frac{hk^2}{1+hk^2} \cdot k^2 |\hat{w}_0(k)| \leq \frac{h}{L^d} \sum_k k^4 |\hat{W}(k)| |\hat{N}_0| \leq hv_4 e^{||\Psi_0||_{\mathcal{D}_0}}$$

and

$$\begin{aligned} ||h^2\underline{L}_h^{-1}(\nabla w_\psi \cdot \nabla\Psi_0)||_{\mathcal{D}_2} &= \frac{h}{L^{2d}} \sum_k \frac{hk^2}{1+hk^2} \sum_q |\hat{\Psi}_0(q)| |\hat{w}_\psi(k-q)| |q \cdot (k-q)| \\ &\leq hv_1 ||\Psi_0||_{\mathcal{D}_1} e^{||\Psi_0||_{\mathcal{D}_0}} \frac{1}{h} \mathcal{E}_1(h||\psi||_{\mathcal{D}_0}) \leq hv_1 ||\Psi_0||_{\mathcal{D}_1} e^{||\Psi_0||_{\mathcal{D}_0}} \frac{1}{h} \mathcal{E}_1(h\mathfrak{b}_0) \end{aligned}$$

(The quantity  $\mathfrak{b}_0$  is defined in the statement of Proposition 5.1.) The result is that we may bound (the sum of) all these terms by an  $h\tilde{A}(h)$  with  $\tilde{A}$  bounded and tending to some  $\tilde{A}(0)$  as  $h \rightarrow 0$ . This leaves – in addition to the  $r_\bullet$  and  $s_\bullet$ -terms – the quantity  $h^2(\nabla\psi \cdot \nabla\Psi_0)$  which we now estimate: Writing  $\psi = \psi_\star + \psi_\bullet$  then

$$\begin{aligned} h^2 \|\underline{L}_h^{-1}(\nabla\psi_\bullet \cdot \nabla\Psi_0)\|_{\mathcal{D}_2} &= \frac{1}{L^{2d}} \sum_{k,q} \frac{h^2 k^2}{1+hk^2} |\hat{\psi}_\bullet(q)| |\hat{\Psi}_0(k-q)| |q \cdot (k-q)| \\ &\leq \frac{1}{2} h^{\frac{3}{2}} \frac{1}{L^{2d}} \sum_{k,q} |\hat{\psi}_\bullet(q)| |\hat{\Psi}_0(k-q)| [q^2 |k-q| + (k-q)^2 |q|] \\ &\leq \frac{1}{2} h^{\frac{1}{2}} [\|h\psi_\bullet\|_{\mathcal{D}_2} \|\Psi_0\|_{\mathcal{D}_1} + h^{\frac{1}{2}} \|h\psi_\bullet\|_{\mathcal{D}_2}^{\frac{1}{2}} \mathfrak{b}_0^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2}]. \end{aligned} \quad (52)$$

In the last step we have used  $\|\psi_\bullet\|_{\mathcal{D}_0} \leq \mathfrak{b}_0$  which is admissible since,  $\mathfrak{b}_0$  is, in fact, an upper bound on  $\|\psi_\star\|_{\mathcal{D}_0} + \|\psi_\bullet\|_{\mathcal{D}_0}$ . We acquire an estimate similar to that in Eq.(52) for the  $\psi_\star$ -term.

We amalgamate our upper bound on  $\|h\psi_\bullet\|_{\mathcal{D}_2}$ :

$$\begin{aligned} \|h\psi_\bullet\|_{\mathcal{D}_2} &\leq h\tilde{A} + \|hr_\bullet\|_{\mathcal{D}_2} + \|hs_\bullet\|_{\mathcal{D}_2} + \frac{1}{2} h^{\frac{1}{2}} [\|h\psi_\bullet\|_{\mathcal{D}_2} \|\Psi_0\|_{\mathcal{D}_1} + h^{\frac{1}{2}} \|h\psi_\bullet\|_{\mathcal{D}_2}^{\frac{1}{2}} \mathfrak{b}_0^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2}] \\ &\quad + \frac{1}{2} h^{\frac{1}{2}} [\|h\psi_\star\|_{\mathcal{D}_2} \|\Psi_0\|_{\mathcal{D}_1} + h^{\frac{1}{2}} \|h\psi_\star\|_{\mathcal{D}_2}^{\frac{1}{2}} \mathfrak{b}_0^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2}] \end{aligned} \quad (53)$$

Let us discuss the term(s) in the last line of the above display: Recalling that we are, in essence, trying to *prove*  $\|h\psi_\star\|_{\mathcal{D}_2} \geq \|h\psi_\bullet\|_{\mathcal{D}_2}$ , if the last terms exceed the corresponding terms just preceding, (that have  $\psi_\star$  replaced by  $\psi_\bullet$ ) we are done. Moreover, if  $h^{\frac{1}{2}} \|h\psi_\bullet\|_{\mathcal{D}_2}^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2} \mathfrak{b}_0^{\frac{1}{2}} \geq \|h\psi_\bullet\|_{\mathcal{D}_2} \|\Psi_0\|_{\mathcal{D}_1}$  this would imply  $\|h\psi_\bullet\|_{\mathcal{D}_2} \leq \mathfrak{b}_\bullet h$  for some generic  $\mathfrak{b}_\bullet$  depending only on  $\mathfrak{D}$ . Once  $\|h\psi_\bullet\|_{\mathcal{D}_2}$  is of order  $h$ , it is no longer important whether or not it exceeds  $\|h\psi_\star\|_{\mathcal{D}_2}$ . Thus, there is no loss of generality if we proceed under both assumptions replacing the two bracketed terms in the above display by  $2h^{\frac{1}{2}} [\|h\psi_\bullet\|_{\mathcal{D}_2} \|\Psi_0\|_{\mathcal{D}_1}]$ . Thus we arrive at the tentative estimate

$$(1 - 2h^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2}) \|h\psi_\bullet\|_{\mathcal{D}_2} \leq h\tilde{A} + \|hr_\bullet\|_{\mathcal{D}_2} + \|hs_\bullet\|_{\mathcal{D}_2} \quad (54)$$

Similarly, we may assume that, as discussed in Claim A<sub>1</sub>, the quantity  $p_0$  does not exceed  $ah^{-\frac{1}{2}}$  since otherwise, automatically,  $\|hr_\bullet\|_{\mathcal{D}_2} + \|hs_\bullet\|_{\mathcal{D}_2}$  is dominated by  $\|h\psi_\star\|_{\mathcal{D}_2}$  and the inequality in Eq.(54) becomes one of the type desired when  $\|h\psi_\star\|_{\mathcal{D}_2}$  is relatively large. Thus our tentative estimate may be rewritten

$$(1 - 2h^{\frac{1}{2}} \|\Psi_0\|_{\mathcal{D}_2}) \|\psi_\bullet\|_{\mathcal{D}_2} \leq hA + (C_r + C_s) \|hL_h^{-1}\Psi_0\|_{\mathcal{D}_3}$$

where  $A$  has been modified from  $\tilde{A}$  by the addition of  $(c_r + c_s)$ .

The conclusion is now inevitable. Recall from Claim A<sub>2</sub> that if the final term on the right exceeds  $\|h\psi_\star\|_{\mathcal{D}_2}$  then both terms (and hence all terms) are of order  $h$ . Otherwise, it is bounded by  $\|h\psi_\star\|_{\mathcal{D}_2}$  and again we have an inequality of the sort desired where  $\|h\psi_\star\|_{\mathcal{D}_2}$  is relatively large.  $\square$



To summarize, so far, we have:

**Corollary 5.4** *Consider Eq.(22) with all elements of  $\mathfrak{D}$  finite. Then there is some  $h_0 = h_0(\mathfrak{D})$  such that for all  $h < h_0$ :*

- i) There is a classical solution  $N_1 = e^{\Psi_1}$  which is bounded below;*
- ii)  $\|\Psi_1\|_{\mathcal{D}_1} - \|\Psi_0\|_{\mathcal{D}_1}$  and  $\|N_1 - N_0\|_{\infty}$  are bounded from above by a constant depending only on the elements of  $\mathfrak{D}$  times  $h$ .*

*Proof.* Most of this follows from the above: indeed,  $|N_1 - N_0| \leq N_0[e^{h b_0} - 1]$  while the lower bound on  $N_1$  certainly follows since  $\Psi_1$  is continuous.  $\square$

## 5.5 Viability of Iterations

For  $h$  sufficiently small, we may envision a few runs of the process. This will provide an updated version of  $\mathfrak{D}$  in which some of the parameters – the mutable parameters – have changed. And, if  $h$  is still small enough this will allow (even according to the bounds) further iterations of the process. In any case if  $k$  iterations of the process are allowed, let us denote by  $\mathfrak{D}_t$  the current values of the parameters where  $(k-1)h \leq t < kh$ ; the original  $\mathfrak{D}$  will thus be denoted by  $\mathfrak{D}_0$ . Here, let us introduce the notion of *viability*:

**Definition 5.5.** Let  $\mathfrak{D}_t$  be defined as above and  $h$  considered fixed. Then the process is deemed to be *viable* for  $h$  if, on the basis of the bounds derived in the preceding two subsections, not only does  $\mathfrak{D}_t$  permit an iteration of the process, but also, still on the basis of these estimates for elements of  $\mathfrak{D}_{t+h}$ , an *additional* iteration is possible.

It is noted that given the elements of  $\mathfrak{D}$ , if  $h$  is sufficiently small, the process *will* be viable. However, this is far from what is needed since we must consider many iterations of the process. The following represents a midway goal of this appendix:

**Proposition 5.6** *Consider the setup encoded in Eq.(22) as has been described. Then there exists a strictly positive  $T = T(\mathfrak{D}_0)$  such that for all  $h$  sufficiently small, the process is viable up till time  $T$ , i.e., the elements of  $\mathfrak{D}_T$  allow for continued iteration of the process.*

It is reemphasized that whenever  $h$  is small enough so that the above statement holds, the conclusion pertains to the order of  $Th^{-1}$  iterations of the process.

*Proof.* Let  $H > 0$  denote a number which is larger than all the mutable parameters in  $\mathfrak{D}_0$  – and indeed might be regarded as considerably larger. After an iteration of the process, assuming  $h$  is small enough to allow such, the mutable parameters will, in all likelihood, have changed (perhaps some for the better). So let us thus define  $\mathbb{H}(H, h)$  so that  $h\mathbb{H}$  is maximum upward change of these mutable parameters, according to the

bounds derived, were they all equal to  $H$  in the first place. Due to monotonicity based on inefficiency, it is clear that if in  $\mathfrak{D}_t$  all mutable parameters are less than or equal to  $H$ , then in  $\mathfrak{D}_{t+h}$  none of them exceed  $H + h\mathbb{H}(H, h)$ . Moreover, it is clear that the  $h \rightarrow 0$  limit of  $\mathbb{H}(H, h)$  is finite, i.e.,  $\mathbb{H}(H, h)$  may be considered to be uniformly bounded.

Now consider  $\mathbb{H}(2H, \cdot)$  and let  $h_2^\dagger$  be small enough so that for all  $h \leq h_2^\dagger$ , provided all mutable parameters in  $\mathfrak{D}$  do not exceed  $2H$ , the process is still viable. I.e., informally, if  $2H$  is “small enough for  $h_2^\dagger$ , then so is  $2H + h_2^\dagger\mathbb{H}(2H, h_2^\dagger)$ ”. Finally, let

$$\mathbb{H}_2^\dagger = \sup_{h < h_2^\dagger} \mathbb{H}(2H, h).$$

The following is now clear: Starting at  $\mathfrak{D}_0$  – with all mutable parameters less than  $H$ , and  $h \leq h_2^\dagger$  we may certainly continue until – according to the derived bounds – one of our mutable parameters reach  $2H$ . This implies there will be at least  $m$  permitted iterations of the process where  $m$  is the largest integer smaller than  $h^{-1}H/\mathbb{H}_2^\dagger$ , i.e.,  $\tau \gtrsim H/\mathbb{H}_2^\dagger$ .  $\square$

It might be envisioned that going to smaller and smaller time steps will allow for indefinite extension of the simulation times. While this is true, and the subject of our next proposition, this cannot be proved on the basis of the bounds on the process that have been so far derived. Indeed, on adhering to the above, in the  $h \rightarrow 0$  limit we would anticipate the bound on  $H$  provided by

$$\frac{dH}{dt} = \mathbb{H}(H, 0).$$

However, such an equation would diverge in finite time as indeed would a “more accurate” equation/bound involving all mutable parameters separately. The needed additional ingredient is provided by the convergence to and the properties of the limiting Eq.(6).

**Proposition 5.7** *Let  $T > 0$  be arbitrary. Then there exists  $h_T > 0$  such that for all  $h \leq h_T$ , the process described by Eq.(22) survives at least up till time  $T$  – that is to say the order of  $h^{-1}T$  iterations.*

*Proof.* The proof relies on the fact that the continuous time equation, Eq.(4) lasts indefinitely and enjoys smoothing properties. In particular, at positive times the functions  $\Psi$  etc., have their  $n$ th derivatives in  $L^1(\mathbb{T}_L^d)$  for all  $n$  [5], hence all the  $\mathcal{D}_k$ -norms are finite. Of course for the purposes of this proof, we are only concerned with the  $\mathcal{D}_0$  thru  $\mathcal{D}_2$  norms and their roles as elements of  $\mathfrak{D}$ .

Consider  $T > 0$ , our fixed macroscopic time. Let  $t_0 > 0$  – but less than the  $\tau(\mathfrak{D}_0)$  featured in Proposition 5.6 – and  $t_1 > T$ . We define  $\beta$  to be the supremum of

the continuous time version of the relevant  $\mathcal{D}_0$ ,  $\mathcal{D}_1$  and  $\mathcal{D}_2$  norms. Since, in this proof, both  $h$  and times will be varying, we shall indicate the former by bracketed superscripts and the latter by subscripts indicating macroscopic times. Thus, e.g.,  $\Psi_t^{[h]}$  denotes the function “ $\Psi$ ” obtained after  $k$  iterations of the process with time step  $h$  for time  $t$  if we have  $t$  the range  $hk \leq t < h(k+1)$ .

Let us operate under the assumption that the statement of this proposition is false for the time  $T$ . Let  $H \gg \beta$  be a quantity similar to that employed in Proposition 5.6 and let us define  $\tau_H^\dagger$  and  $\tau_{2H}^\ddagger$  to be convenient times when the largest of the mutable elements of  $\mathfrak{D}_t^{[h]}$  are in the range  $[H, 2H]$ . Precise definitions are as follows:

- $\tau_{2H}^\ddagger(h)$  is such that at this time, the maximal element of the associated  $\mathfrak{D}$  is less than  $2H$  but at time  $\tau_{2H}^\ddagger + h$ , some element exceeds  $2H$  for the first time in the process;
- $\tau_H^\dagger(h)$  is such that at this time, some element of the set  $\mathfrak{D}$  exceeds  $H$ . This condition will persist till (at least)  $\tau_{2H}^\ddagger$ , however at time  $t = \tau_H^\dagger - h$ , all the mutable elements of  $\mathfrak{D}_t^{[h]}$  were below  $H$ .

The assumed falsehood of the statement of this proposition implies that these times exist, are well defined and satisfy,

$$\limsup_{h \rightarrow 0} \tau_{2H}^\ddagger \leq T$$

Thus we have a family of compact intervals  $[\tau_H^\dagger(h), \tau_{2H}^\ddagger(h)]$  which, by the arguments of Proposition 5.6 are non-empty and, indeed, of size uniformly bounded below. Let us start by restricting to a subsequence of  $h$ 's – which we will not adorn with further labels – in which the intersection of these subsequent intervals contains an interval to which we will restrict our attention. Now, it is emphasized, the totality of all iterations in the subsequence under consideration is countable.

In the intersection of the above mentioned regions, the iteration process is certainly viable and hence the results of Proposition 3.8 may be applied. I.e., here we have convergence to the continuum equation. Also  $\|\Psi_t^{[h]}\|_{\mathcal{D}_1}$  and  $\|\Psi_t^{[h]}\|_{\mathcal{D}_2}$  are bounded so these converge weakly (along any  $t_j \rightarrow t, h_j \rightarrow 0$  subsequence) to their continuum values, however  $\|\Psi_t^{[h]}\|_{\mathcal{D}_2} < 2H$  provides a tightness condition for  $\nabla \Psi_t^{[h]}$  – as well as  $\Psi_t^{[h]}$  itself – hence these converge strongly. Thus, further restricting the  $h$ 's if necessary,  $\|\Psi_t^{[h]}\|_{\mathcal{D}_0}, \|\Psi_t^{[h]}\|_{\mathcal{D}_1} < 2\beta$  for all  $t$  and  $h$ . However, since something in the  $\mathfrak{D}_t$ 's must be greater than  $H$  it is evident that we have  $\|\Psi_t^{[h]}\|_{\mathcal{D}_2} > H$ . This implies that these objects are converging weakly but not strongly in  $\mathcal{D}_2$ .

Let us summarize the strategy for the remainder of this proof. We will show that the purported circumstances imply that among the iterative corrections, the dominant term, by far, is  $\psi_\star$  (c.f., Eq.(48) and Eq.(49)). Thence  $\Psi_{t+h}^{[h]}$  is given, in essence, by  $(\Psi_{t+h}^{[h]})_\star$  which, we remind the reader, enjoys a reduction in *all*  $k \neq 0$  Fourier modes.

So, in particular, we will show  $\|\Psi_{t+h}^{[h]}\|_{\mathcal{D}_2} < \|\Psi_t^{[h]}\|_{\mathcal{D}_2}$ , indicating that the time  $\tau_{2H}^\dagger(h)$  is never reached, effecting a contradiction.

In what follows, we shall make statements which, properly speaking hold for all but a finite number of  $h$  and time intervals. We shall abbreviate by saying “for all”, automatically going to subsequences if necessary.

Our first claim is that  $\|\underline{L}_h^{-1}\nabla^2\Psi_t^{[h]}\|_{\mathcal{D}_2}$  (corresponding to the  $\psi_\star$ -term, c.f., Eq(48)) is, in essence, indefinitely large. To this end, let  $\mathcal{Q}$  denote a fixed large number the necessary dimensions of which will be specified eventually. If, we suppose, that for infinitely many terms,

$$\sum_{|q|\leq\mathcal{Q}} q^2|\hat{\Psi}_t^{[h]}(q)| > \frac{1}{2}H$$

then this would imply that any weak  $\mathcal{D}_2$ -limit of  $\Psi_t^{[h]}$  would have  $\mathcal{D}_2$ -norm in excess of  $\beta$ . Thus we have, without loss of generality, that for all  $h$  and  $t$ ,

$$\sum_{|q|>\mathcal{Q}} q^2|\hat{\Psi}_t^{[h]}(q)| \geq \frac{1}{2}H.$$

Now for all  $h$  sufficiently small –  $\mathcal{Q}$  fixed – it is clear that  $k^2/[1+hk^2] > (\frac{1}{2}\mathcal{Q})^2$  whenever  $k > \mathcal{Q}$  and thus  $\|\underline{L}_h^{-1}\nabla^2\Psi_t^{[h]}\|_{\mathcal{D}_2} \gtrsim H\mathcal{Q}^2$ :

$$\|\underline{L}_h^{-1}\nabla^2\Psi_t^{[h]}\|_{\mathcal{D}_2} \geq \sum_{|q|>\mathcal{Q}} \frac{q^2}{1+hq^2} q^2|\hat{\Psi}_t^{[h]}(q)| \geq \frac{1}{8}\mathcal{Q}^2H.$$

This is deemed to be larger than all peripheral terms e.g.,  $c_r$ ,  $c_s$ , etc., which are at most multiples of  $H$ . The only possible difficulties concern the terms  $r_\bullet$  and  $s_\bullet$ . According to one scenario, namely  $p_0 \geq ah^{-\frac{1}{2}}$  (c.f., Claim A<sub>1</sub> – and noting the factor of two) these terms could only account for half of the term  $\|\underline{L}_h^{-1}\nabla^2\Psi_t^{[h]}\|_{\mathcal{D}_2}$  and the remainder is more than sufficient for all else. Otherwise, it is recalled, the added  $\underline{L}_h^{-1}r_\bullet$  and  $\underline{L}_h^{-1}s_\bullet$  terms have  $\mathcal{D}_2$ -norms bounded by

$$(C_r + C_s) \sum_q \frac{q^3}{1+hq^2} |\hat{\Psi}_t^{[h]}(q)|.$$

As for the range  $|q| \leq q_0$  (where we recall  $q_0 = 2(C_r + C_s)$ ) we may bound the corresponding contribution of the above by a multiple – 8 – of  $(C_r + C_s)^3 \|\Psi_t^{[h]}\|_{\mathcal{D}_1}$ . This is deemed to be negligibly small compared to  $\mathcal{Q}^2H$ . In the range  $q_0 < |q| \leq \mathcal{Q}$ , the terms contributing to  $\|\underline{L}_h^{-1}\nabla^2\Psi_t^{[h]}\|_{\mathcal{D}_2}$  dominate their counterparts in the above display and so we may ignore these differing contributions. This leaves us with  $|q| > \mathcal{Q}$  where it may be asserted

$$\frac{q^4 - (C_r + C_s)q^3}{1+hq^2} \geq q^2[(\frac{1}{2}\mathcal{Q})^2 - (C_r + C_s)\mathcal{Q}].$$

This leaves us an overall *excess* at least as large as  $[(\frac{1}{2}\mathcal{Q})^2 - (C_r + C_s)\mathcal{Q}] \times \frac{1}{2}H$ . It is thus seen that for  $\mathcal{Q}$  chosen to be large enough, the increment for  $\|\Psi_t^{[h]}\|_{\mathcal{D}_2}$  on each step of the iteration is negative which establishes the desired contradiction.  $\square$

*Proof of Proposition 3.8, Item(A).* As before, we let  $\Psi_t$  denote the limiting quantity which satisfies the appropriate version of Eq.(22). Recalling the result of Proposition 5.1 that the increment in  $\Psi_t^{[h]}$  is uniformly bounded by a constant times  $h$  (implying uniform continuity in time) it follows from the weak convergence of  $\Psi_t^{[h]}$  that for all  $t$  and for each wavenumber  $q$ ,

$$\hat{\Psi}_t^{[h]}(q) \rightarrow \hat{\Psi}_t(q).$$

Now the fact that  $\|\Psi_t^{[h]}\|_{\mathcal{D}_1}$  is uniformly bounded certainly implies weak convergence in  $\mathcal{D}_1$ . But boundedness of  $\|\Psi_t^{[h]}\|_{\mathcal{D}_2}$  implies strong convergence – throughout the procedure of convergence, only a finite number of modes contribute essentially – and by the above, we identify, mode by mode, exactly what the limit is.

Our final result, uniform convergence in the  $\mathcal{D}_0$ -norm, may be expressed via

$$\lim_{h \rightarrow 0} \sup_{t \in [0, T]} \|\Psi_t - \Psi_t^{[h]}\|_{\mathcal{D}_0} = 0$$

First, let  $h_j$  denote a sequence tending to zero (always below  $h_T$ ) where it may be envisioned that in the above, the superior  $h \rightarrow 0$  limit is achieved. Let  $t_j$  denote an integer time closest to the time where the  $h = h_j$  supremum in the above display is to be found. Since  $\Psi_t$  is, evidently, uniformly ( $\mathcal{D}_0$ ) continuous in time, we may evaluate, without loss of generality,

$$\limsup_{j \rightarrow \infty} \|\Psi_{t_j} - \Psi_{t_j}^{[h_j]}\|_{\mathcal{D}_0}.$$

We let  $t^\dagger = \lim_{j \rightarrow \infty} t_j$  – perhaps along a further subsequence – and then the above limit is seen to be zero by the application of the triangle inequality:

$$0 = \lim_{j \rightarrow \infty} \|\Psi_{t_j} - \Psi_{t^\dagger}\|_{\mathcal{D}_0} = \lim_{j \rightarrow \infty} \|\Psi_{t^\dagger} - \Psi_{t^\dagger}^{[h_j]}\|_{\mathcal{D}_0} = \lim_{j \rightarrow \infty} \|\Psi_{t_j}^{[h_j]} - \Psi_{t^\dagger}^{[h_j]}\|_{\mathcal{D}_0};$$

the final zero because we have seen that, uniformly in  $h$ , with all elements of  $\mathfrak{D}_t$  uniformly bounded,  $\|\Psi_t^{[h]}\|_{\mathcal{D}_0}$  is uniformly continuous in time.  $\square$

We can now extend Corollary 5.4 to arbitrary macroscopic times:

**Corollary 5.8** *Consider Eq.(22) with all elements of  $\mathfrak{D}_0$  finite and let  $T > 0$ . Then there is some  $h_T = h_T(\mathfrak{D})$  such that for all  $h < h_T$  and  $t < T$ :*

- i) There is a classical solution  $N_t^{[h]} = e^{\Psi_t^{[h]}}$  which is bounded below;*
- ii)  $\|\Psi_t^{[h]}\|_{\mathcal{D}_1} - \|\Psi_t^{[h]}\|_{\mathcal{D}_1}$  and  $\|N_t^{[h]} - N_0\|_\infty$  are bounded from above by a constant depending only on the elements of  $\mathfrak{D}$  times  $h$ .*

*In the above, the notation  $N_t^{[h]}$  etc., is as in the proof of Theorem 3.8.*

*Proof.* With the results of Proposition 5.7 etc., in hand, the proof follows *mutates mutants* from the proof of Corollary 5.4.  $\square$

## 6 Appendix B

In this appendix – which is not *essential* for this work but is requisite for completeness – we present the basic properties of the distance function on  $\mathcal{B} \times \mathcal{B}$  (particularly that it actually is a distance).

**Proposition 6.1** *For  $N_0, N_1 \in \mathcal{B}$ , consider  $\mathbb{D}^2(N_0, N_1)$  as given in Eq.(13). Then the infimum in this equation is achieved by minimizing among velocity fields that are derived from potentials.*

*Proof.* Let  $N_t$  denote a path in  $\mathcal{B}$  from  $N_0$  to  $N_1$  as described in Eq.(12) which we suppose is driven advectively by the field  $V \in \mathcal{V}(N_0, N_1)$ :

$$\frac{\partial N_t}{\partial t} = -\nabla \cdot (N_t V) - \Omega_{N_t} \mathbb{I}_{\nabla}(V).$$

Now let  $\phi$  denote a velocity potential which also produces the path  $N_t$  (as in the derivations following (12)):

$$\frac{\partial N_t}{\partial t} = \nabla \cdot (N_t \nabla \phi) - \Omega_{N_t} \phi.$$

Then, with apologies for minus signs in the above and in the forthcoming, multiplying both of the above by  $-\phi$  and integrating by parts, we have, for a.e.  $t$ ,

$$\langle \nabla \phi, \nabla \phi \rangle_{N_t} = \langle -\nabla \phi, V \rangle_{N_t};$$

I.e., the difference between  $V$  and  $-\nabla \phi$  is orthogonal to  $\nabla \phi$ . Thus

$$\begin{aligned} \langle V, V \rangle_{N_t} &= \langle V + \nabla \phi, V + \nabla \phi \rangle_{N_t} - 2\langle V, \nabla \phi \rangle_{N_t} - \langle \nabla \phi, \nabla \phi \rangle_{N_t} \\ &= \langle V + \nabla \phi, V + \nabla \phi \rangle_{N_t} + \langle \nabla \phi, \nabla \phi \rangle_{N_t} \\ &\geq \langle \nabla \phi, \nabla \phi \rangle_{N_t}. \end{aligned} \tag{55}$$

Thence, at least from the perspective of a minimization program, we are better off using the gradient fields.  $\square$

Here we establish the so-called indiscernible property of  $\mathbb{D}(\cdot, \cdot)$  as stated below. In the follows, we shall actually make some use of the finite range assumption on the interaction  $W(\cdot)$ .

**Proposition 6.2** *Let  $N_0, N_1 \in \mathcal{B}$  with  $N_0 \neq N_1$ . Then*

$$\mathbb{D}^2(N_0, N_1) \neq 0.$$

*Proof.* We first claim that

$$\Omega_N \leq e^{\frac{1}{2}|\mu - w_N|} \cdot \frac{1}{2}(1 + N).$$

Indeed, writing  $\Omega_N = N^{\frac{1}{2}} \sinh(\frac{1}{2}\Phi_N) / \frac{1}{2}\Phi_N \leq N^{\frac{1}{2}} \cosh \frac{1}{2}\Phi_N$ , the result follows immediately.

Next, for  $x_0 \in \mathbb{T}_L^d$ , let  $B_a(x_0)$  denote the ball of radius  $a$  centered at  $x_0$  and here  $a$  denotes the interaction radius of  $W$ . Let  $\varphi(x)$  denote any positive  $\mathcal{C}^2$  function which is identically one on  $B_a(0)$  and decreases to zero outside, specifically –say– in  $B_{2a}(0) \setminus B_a(0)$ . Let us further assume that  $|\nabla \varphi|^2 \leq g_\varphi \varphi$  for some constant  $g_\varphi$ . For brevity, we use  $\varphi_{x_0}(x) := \varphi(x - x_0)$ . For  $N \in \mathcal{B}$  we define

$$p_N(x_0) := \int_{\mathbb{T}_L^d} \varphi_{x_0} N dx$$

which, it is noted, is an upper bound on the  $N$ –measure of  $B_a(x_0)$  (and a lower bound on the  $N$ –measure of  $B_{2a}(x_0)$ ). Moreover, it is noted that  $p_N(x)$  is a continuous function of  $x$ . Finally, for  $N$  fixed, we have

$$|w_N(x_0)| \leq w_0 \cdot p_N(x_0)$$

With  $w_0$  the  $\mathcal{C}_0$ –norm of  $W$ . Indeed,

$$|w_N(x_0)| = \left| \int_{\mathbb{T}_L^d} W(x_0 - y) N_t(y) dy \right| \leq \int_{\mathbb{T}_L^d} |W(x_0 - y)| N_t(y) dy \leq w_0 N_t(B_a(x_0))$$

and we use the previously mentioned upper bound.

Assuming  $\mathbb{D}^2(N_0, N_1) = 0$ , let  $N_t^{(k)}$  be a minimizing sequence of paths in  $\mathcal{B}$  connecting  $N_0$  and  $N_1$ . We denote by  $\Psi_t^{(k)}$  the associated driving potentials. By our assumption, it is the case that  $\varepsilon_k(t)$  defined by

$$\varepsilon_k^2(t) := - \int_{\mathbb{T}_L^d} \Psi_t^{(k)} \frac{\partial N_t^{(k)}}{\partial t} dx = \langle \nabla \Psi_t^{(k)}, \nabla \Psi_t^{(k)} \rangle_{N_t}$$

satisfies

$$0 = \lim_{k \rightarrow \infty} \int_0^1 \varepsilon_k^2(t) dt.$$

For  $x \in \mathbb{T}_L^d$ ,  $t \in [0, 1]$  and  $k$  an integer let us abbreviate  $p_{N_t^{(k)}}(x)$  by  $p_{t,k}(x)$ . It is observed that (for fixed  $k$ )  $p_{t,k}(x)$  is a continuous function on  $[0, 1] \times \mathbb{T}_L^d$ . Indeed, for fixed  $x_0$  we can estimate the evolution of  $p_{t,k}(x_0)$ .

We have

$$-\frac{d}{dt} p_{t,k}(x_0) = \langle \nabla \varphi_{x_0}, \nabla \Psi_t^{(k)} \rangle_{N_t^{(k)}}$$

so that

$$\left| \frac{d}{dt} p_{t,k}(x_0) \right| \leq \varepsilon_k(t) \langle \nabla \varphi_{x_0}, \nabla \varphi_{x_0} \rangle_{N_t^{(k)}}^{\frac{1}{2}};$$

the above for a.e.  $t$ . We now examine  $\langle\langle \nabla \varphi_{x_0}, \nabla \varphi_{x_0} \rangle\rangle_{N_t^{(k)}}$ . As for the gradient term, this is agreeably bounded in terms of  $\varphi_{x_0}$  itself:

$$\int_{\mathbb{T}_L^d} |\nabla \varphi_{x_0}|^2 N_t^{(k)} dx \leq g_\varphi \cdot p_{t,k}$$

The second term still contains the non-local  $w_N(x)$  which, even with the prior estimates still involves an integration in  $B_a(x_0)$ . Let us temporarily be content with

$$\int_{\mathbb{T}_L^d} \varphi_{x_0}^2 \Omega_{N_t^{(k)}}(x) dx \leq \frac{1}{2} \int_{\mathbb{T}_L^d} e^{\frac{1}{2}|\mu - w_N|} \varphi_{x_0}^2 (1 + N_t^{(k)}) dx \leq \frac{1}{2} e^{\frac{1}{2}\mu} \int_{\mathbb{T}_L^d} \varphi_{x_0}^2 e^{\frac{1}{2}w_0 \cdot p_{t,k}(x)} (1 + N_t^{(k)}) dx.$$

Now, consider  $I_0$  defined by

$$I_0 = \max_{x \in \mathbb{T}_L^d} p_{k,0} \equiv \max_{x \in \mathbb{T}_L^d} \int \varphi_x N_0 dx$$

which is manifestly independent of  $k$ .

It is clear that for any given  $x$  if we define

$$t_k^\sharp(x) := \sup\{t \in [0, 1] \mid p_{k,t}(x) < 2I_0\}$$

then  $t_k^\sharp(x) > 0$ . Moreover, it can easily be established using the continuity of  $p_{k,\cdot}(\cdot)$  that

$$t_k^\flat := \inf_{x \in \mathbb{T}_L^d} t_k^\sharp(x)$$

is strictly positive. But *a priori*  $t_k^\flat$  is not necessarily uniformly positive in  $k$ ; notwithstanding we will show, under the hypothesis  $\mathbb{D}^2(N_0, N_1) = 0$ , that for all  $k$  sufficiently large,  $t_k^\flat \equiv 1$ .

Indeed, provided  $t < t_k^\flat$ , we may estimate the final term in the estimate prior to the definition of  $I_0$ :

$$\int \varphi_{x_0}^2 \Omega_{N_t^{(k)}}(x) dx \leq \frac{1}{2} e^{\frac{1}{2}|\mu| + w_0 I_0} \int \varphi_{x_0}^2 (1 + N_t^{(k)}) dx \leq c_1 e^{c_2 I_0} (c_3 + I_0)$$

for finite constants  $c_1 \dots c_3$  which do not depend on  $k$  or  $t$ .

So, we may write, for  $t < t_k^\flat$ ,

$$p_{k,t}(x_0) \leq p_{k,0}(x_0) + [c_4 I_0 + c_1 e^{c_2 I_0} (c_3 + I_0)]^{\frac{1}{2}} \cdot \int_0^t \varepsilon_k(t) dt,$$

with  $c_4$  similar to the above  $c$ 's. It is noted that the first term on the right is independent of  $k$  and bounded by  $I_0$ . Let  $\gamma_k$  be defined by

$$[c_4 I_0 + c_1 e^{c_2 I_0} (c_3 + I_0)]^{\frac{1}{2}} \cdot \int_0^1 \varepsilon_k(t) dt := \gamma_k I_0$$

where it is noted that the upper limit of the integration is  $t = 1$ . We have, for all  $k$  sufficiently large that  $\gamma_k < 1$  and we have at  $t = t_k^\flat$  that for any  $x$ ,

$$p_{k,t_k^\flat} \leq I_0(1 + \gamma_k)$$



which necessitates  $t_k^b = 1$ . Further, as  $k \rightarrow \infty$ , we find that for any  $x$ ,  $p_{k,t}(x)$  is pinned at its initial value – which essentially proves the desired result. But let us anyway proceed:

We note on the basis of the previous analysis that the quantity  $\Omega_{N_{t,k}}$  is bounded by  $e^{\frac{1}{2}|\mu|}e^{w_0 I_0}(1 + N_{t,k})$  meaning that for any positive (and, e.g.,  $\mathcal{C}^2$ ) function  $f$ ,

$$\int f \Omega_{N_{t,k}} dx \leq e^{\frac{1}{2}|\mu|}e^{w_0 I_0} \int f(1 + N_{t,k}) dx.$$

In particular, with  $f \equiv 1$  we find that the total mass,  $\mathbb{M}_{t,k}$  satisfies the differential inequality

$$\frac{d\mathbb{M}_{t,k}}{dt} \leq e^{\frac{1}{2}|\mu|}e^{w_0 I_0} \varepsilon_k(t) [L^d + \mathbb{M}_{t,k}]^{\frac{1}{2}}.$$

Defining

$$\vartheta_k := \int_0^1 \varepsilon_k(t) dt \propto \gamma_k$$

and noting  $\vartheta_k \rightarrow 0$  as  $k \rightarrow \infty$  we learn

$$\mathbb{M}_{t,k} \leq \mathbb{M}_0 + c \cdot \vartheta_k$$

where  $c$  is another constant depending e.g., on  $\mathbb{M}_0$ , the total volume and other particulars but is independent of  $k$  and  $t$ .

The proof is now easily finished. Let  $\eta$  denote any  $\mathcal{C}^2$  function. Then for any  $k$ ,

$$\int_{\mathbb{T}_L^d} \eta(N_0 - N_1) dx = \int_{\mathbb{T}_L^d} \langle \nabla \eta, \nabla \Psi_{k,t} \rangle_{N_{t,k}} dt$$

and (for  $k$  sufficiently large) the right hand side is bounded by  $\|\eta\|_{\mathcal{C}^2} \cdot \vartheta_k \cdot [c_5 \mathbb{M}_0 + c_6]^{\frac{1}{2}}$  (with  $c_5$  and  $c_6$  similar to earlier  $c$ 's). Letting  $k \rightarrow \infty$ , we learn

$$\int \eta dN_0 = \int \eta dN_1$$

which, since  $\eta$  is arbitrary, establishes  $N_0 = N_1$  □

**Theorem 6.3** *The function  $\mathbb{D}(\cdot, \cdot)$  defines a distance on  $\mathcal{B}$ .*

*Proof.* Letting  $N_0, N_1 \in \mathcal{B}$ , to help with the abbreviation of the forthcoming, let us name by  $\mathbb{E}$  the functional whose infimum produces  $\mathbb{D}(N_0, N_1)$ . By Proposition 6.1 we may regard *potentials* as the arguments of this functional:

$$\mathbb{E}^2(Q) = \mathbb{E}_{N_0, N_1}^2(Q) = \int_0^1 \langle \nabla Q, \nabla Q \rangle_{N_t} dt = \int_0^1 \int_{\mathbb{T}_L^d} N_t |\nabla Q|^2 + \Omega_{N_t} Q^2 dx dt$$

where it is noted but notationally suppressed that  $-\nabla Q \in \mathcal{V}(N_0, N_1)$  (where  $\mathcal{V}$  is defined just below Eq.(11) with the adjustable  $\kappa$  built into the *definition* of the potential). We may also make the trivial addition – as mentioned and utilized elsewhere in

this text – of allowing the potential to achieve  $N_1$  at times  $T$  other than  $t = 1$  in which case the functional becomes  $T \int_{[0,T]} \langle \nabla Q, \nabla Q \rangle_{N_t} dt$ .

Beyond the indiscernible property established above, we must show that  $\mathbb{D}(N_0, N_1) = \mathbb{D}(N_1, N_0)$  and establish the triangle inequality. The first follows immediately from “time reversal symmetry”; e.g., on  $[0, 1]$ ,  $t' = 1 - t$ ,  $K(t') = -Q(1 - t')$  gives  $\mathbb{E}_{N_0, N_1}^2(Q) = \mathbb{E}_{N_1, N_0}^2(K)$  and the result follows.

As for the triangle inequality, we shall be as succinct as possible since the result follows a transcription of the standard derivation from Riemannian geometry. We first define  $\underline{\mathbb{E}}(Q)$  by taking the square root of the integrand in the definition of  $\mathbb{E}^2$  when the time interval is  $[0, 1]$  and/or shedding the time prefactor and integrating up to the arrival time at  $N_1$ . We denote the corresponding minimized object by  $\underline{\mathbb{D}}(N_0, N_1)$ . It is noted that  $\underline{\mathbb{E}}(Q)$  is invariant under the full set of time changes:  $t \rightarrow \tau(t)$ ,  $Q(t) \rightarrow K(\tau) = \vartheta(\tau)Q(t(\tau))$  with  $\vartheta = \frac{dt}{d\tau}$  has  $\mathbb{E}(Q) = \mathbb{E}(K)$  with  $K$  *legitimately* driving  $N_0$  to  $N_1$  on the interval  $[0, \tau(T)]$ .

By convexity we have  $\mathbb{E}^2(Q) \geq [\underline{\mathbb{E}}(Q)]^2$  and so  $\mathbb{D}^2(N_0, N_1) \geq [\underline{\mathbb{D}}(N_0, N_1)]^2$ . On the other hand, defining  $\underline{\mathbb{E}}_t := \int_{[0,t]} \langle \nabla Q, \nabla Q \rangle_{N_{t'}}^{\frac{1}{2}} dt'$ ;  $t \leq T$ , and reparameterizing with  $\tau = \tau(t) = \underline{\mathbb{E}}_t$ ,  $K = [\frac{d\underline{\mathbb{E}}_t}{dt}]^{-1} Q(t(\tau))$ , it is seen that, in the new variables, all integrands are identically one. And so we have

$$\underline{\mathbb{E}}^2(Q) = \underline{\mathbb{E}}^2(K) = \underline{\mathbb{E}}(K) \int_0^{\underline{\mathbb{E}}_T} d\tau = \tau(T) \int_0^{\tau(T)} \langle \nabla K, \nabla K \rangle_{N_\tau} d\tau = \mathbb{E}^2(K).$$

Taking the infimum over  $K$ 's (or  $Q$ 's) we arrive at  $\mathbb{D}(N_0, N_1) = \underline{\mathbb{D}}(N_0, N_1)$ . The triangle inequality is immediate since, for  $N_0, N_1, N_2 \in \mathcal{B}$  we can attempt to minimize  $\underline{\mathbb{E}}_{N_0, N_2}(\cdot)$  by considering paths which “go through”  $N_1$  on the way to  $N_2$  and so we conclude that  $\mathbb{D}(N_0, N_2) \leq \mathbb{D}(N_0, N_1) + \mathbb{D}(N_1, N_2)$ .  $\square$

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